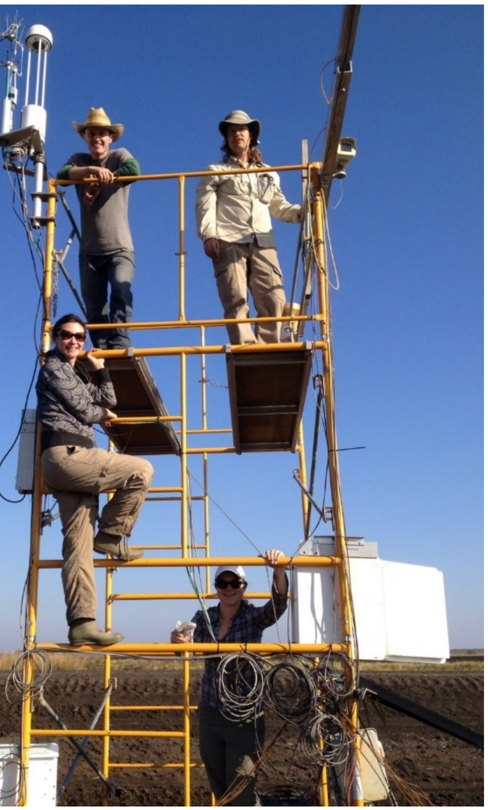


Using a Hierarchy of Modeling Approaches to Mine a Rich Dataset of Greenhouse Gas Fluxes Measurements: Experiences Derived from a Meso-network of Agricultural and Restored Wetland Sites in the Peat-Rich Delta of California

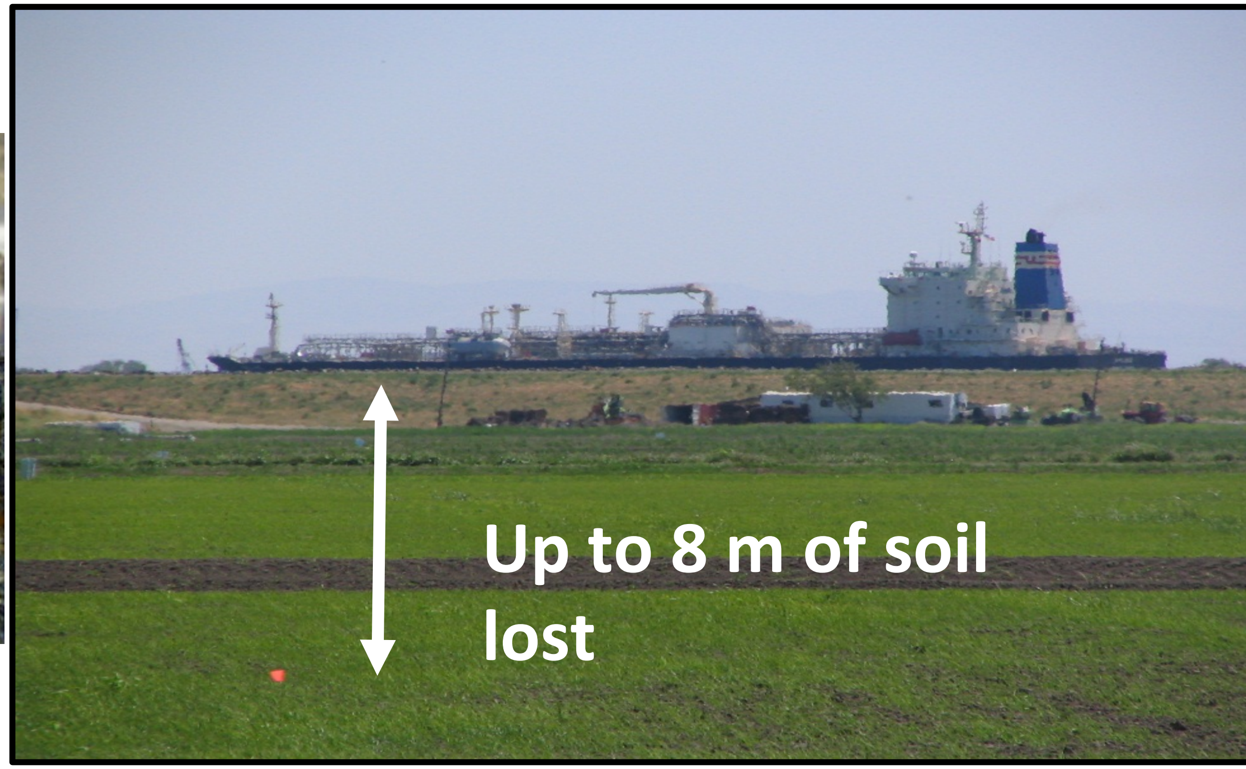
Dennis Baldocchi, Patty Oikawa, Sara Knox, Cove Sturtevant, Jaclyn Hatala, Matteo Detto, Joe Verfaillie

University of California, Berkeley

International Conference on Soil Modeling
Austin, TX, March, 2016

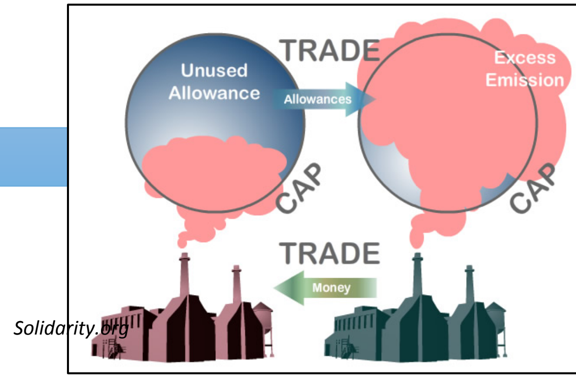
The Problem: Oxidation and Subsidence of Peatland

PEAT SOIL >18m



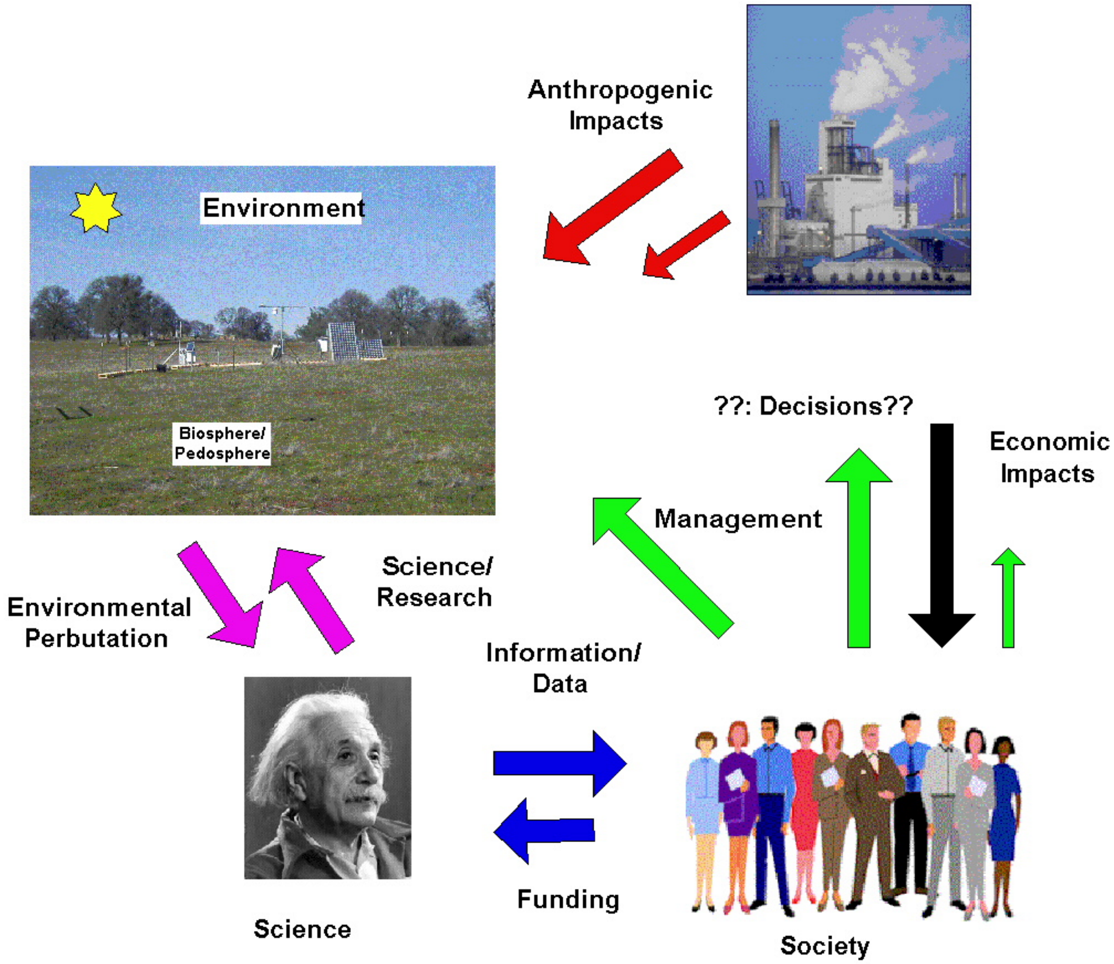
- 100+ yr loss of ~ 1 Pg of C
- Water Source and Conduit for 20+ million Californians

Solution: Restore Wetlands, Sell Carbon Credits to Cap and Trade Mar



Can We Re-Convert the Land to a Carbon Sink by Replacing Agriculture with Restored Wetlar
What are the Unintended Costs of Flooding the Land, in terms of Greenhouse Gas productior
Can We Estimate Net Carbon Fluxes with Simple Models and Inputs?

Approach: Measure and Model Greenhouse Gas Fluxes to Assess Efficacy of Land Use Change and Unintended Consequences



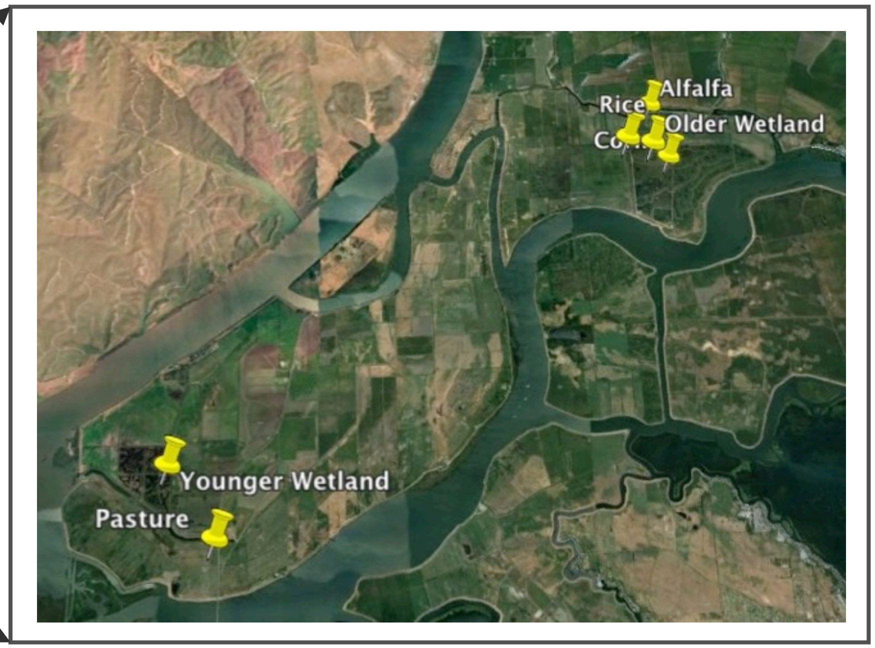
Use Science to Better Inform Policy and Societal Actions

Outline

- Test the Performance of a Hierarchy of Simple to Complex CO_2 and CH_4 Flux Models for Applied and Basic Problems and Questions
- Deconstruct Model Performance for the Plant and Soil Compartments
- Use Emerging Math Methods to Discover New Information in our Data about Covariances, Leads/Lags and Pulses between Fluxes and Biophysical Variables across a Spectrum of Time Scales
  - Guide to Future Model Evolution

Venue: UC Berkeley Meso-Network of Eddy Covariance Flux Stations

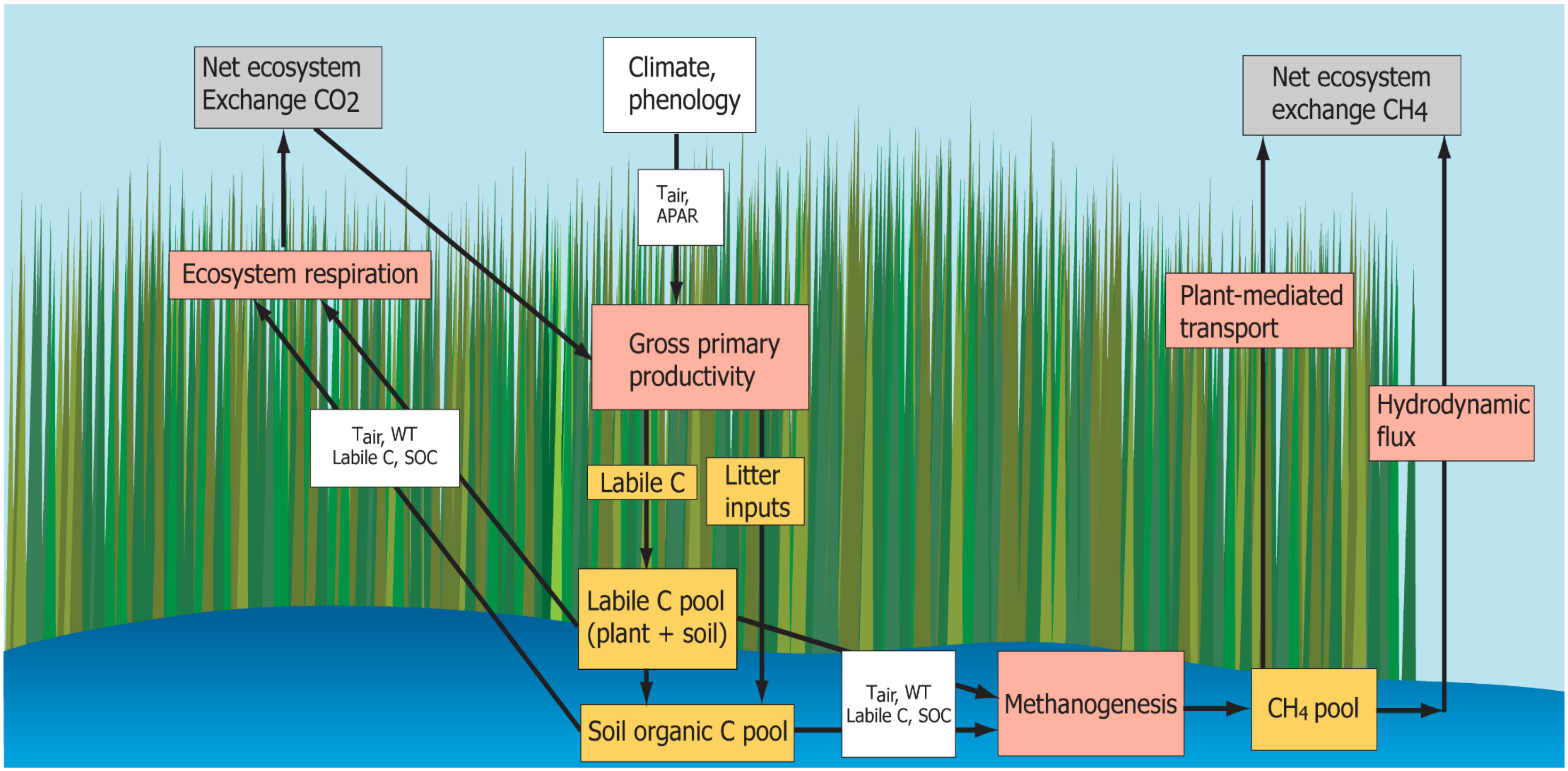
San Francisco Estuary Institute-Aquatic Science Center, 2012



Models Used

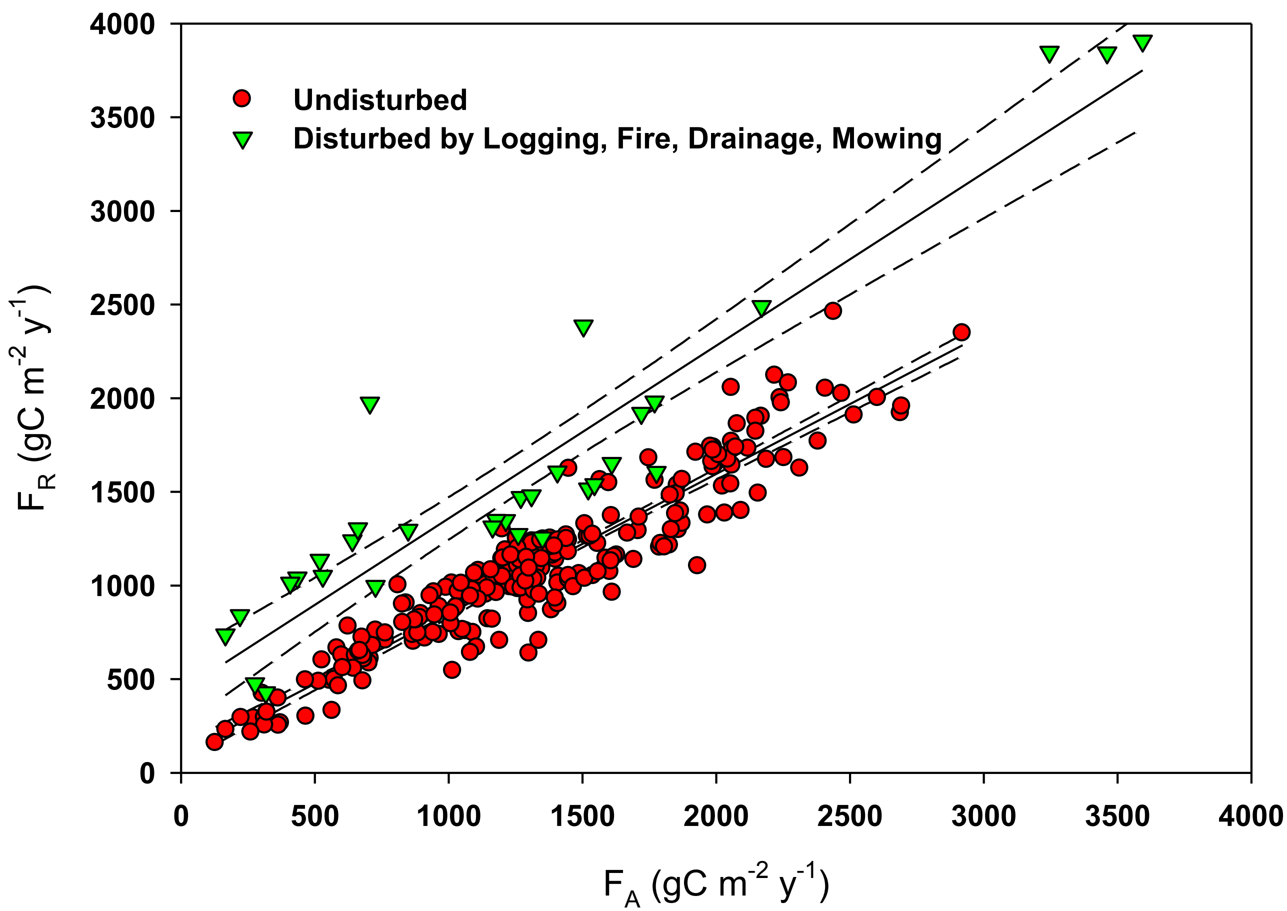
- Dynamics Pool Models
  - Fit parameters with Flux measurements and Bayesian Statistics to produce simple models for assessment of Greenhouse Gas Budgets for Carbon Markets
- Process-Based and Mechanistic Biophysical Models, CANVEG
  - Understand the fundamental processes Modulating C Exchange of Plant and Soil Compartments Fluxes
  - Predict future fluxes
- Statistical/Empirical Models
  - Artificial Neural Networks (ANN) to Gap Fill Flux Data and Compute Daily and Annual Integrals
  - Mutual Information Theory, Granger Causality and Artificial Neural Networks to discover Modulation of Fluxes by Biophysical Variables at Different Time Scales (hourly, daily, weekly, seasonal, annual), Roles of Non-Linear Interactions and Leads and Lags

PEPRMT Model: Soil Fluxes are Coupled to Plants



wa et al. in prep, JGR Biogeosci

Premise: Ecosystem Respiration Scales Tightly with Ecosystem Photosynthesis



Baldocchi, Austral J Botany 2008

ey Algorithms

Light Use Efficiency Model for Photosynthesis

$$GPP = LUE * APAR * f(T_k)$$

Boltzmann Function for Temperature Kinetics

$$f(T_k) = \frac{H_d \, exp(\frac{(H_a(T_k - T_{opt})}{T_k \, R \, T_{opt}})}{H_d - (1 - exp(\frac{(H_d(T_k - T_{opt})}{T_k \, R \, T_{opt}})}$$

ichaelis-Menten Enzyme Kinetics for
ration and
ethane Production and Oxidation

$$R_{eco} = \left(\frac{V_{max,SOC}\left[C_{SOC}\right]}{K_{m,SOC} + \left[C_{SOC}\right]} + \frac{V_{max,Labile}\left[C_{Labile}\right]}{K_{m,\,Labile} + \left[C_{Labile}\right]} \right) * (1 - f\left(WT\right)$$

$$R_{CH_4} = \left(\frac{V_{max,SOC}\left[C_{SOC}\right]}{K_{m,SOC} + \left[C_{SOC}\right]} + \frac{V_{max,Labile}\left[C_{Labile}\right]}{K_{m,\,Labile} + \left[C_{Labile}\right]} \right) * (1 - f\left(WT\right)$$

$$O_{CH_4} = \left(\frac{V_{max,CH4}\left[C_{CH4}\right]}{K_{m,CH4} + \left[C_{CH4}\right]} \right) * (1 - f\left(WT\right)$$

odel Data Fusion

Bayes Theorem

$$p(\theta_{1,}\theta_2 \mid x, y) \propto p(\theta_1 \mid y, \theta_2, x) \cdot p(\theta_1) \cdot p(\theta_2)$$

Parameters, given data | Likelihood, Data model | Priors, Parameter Model

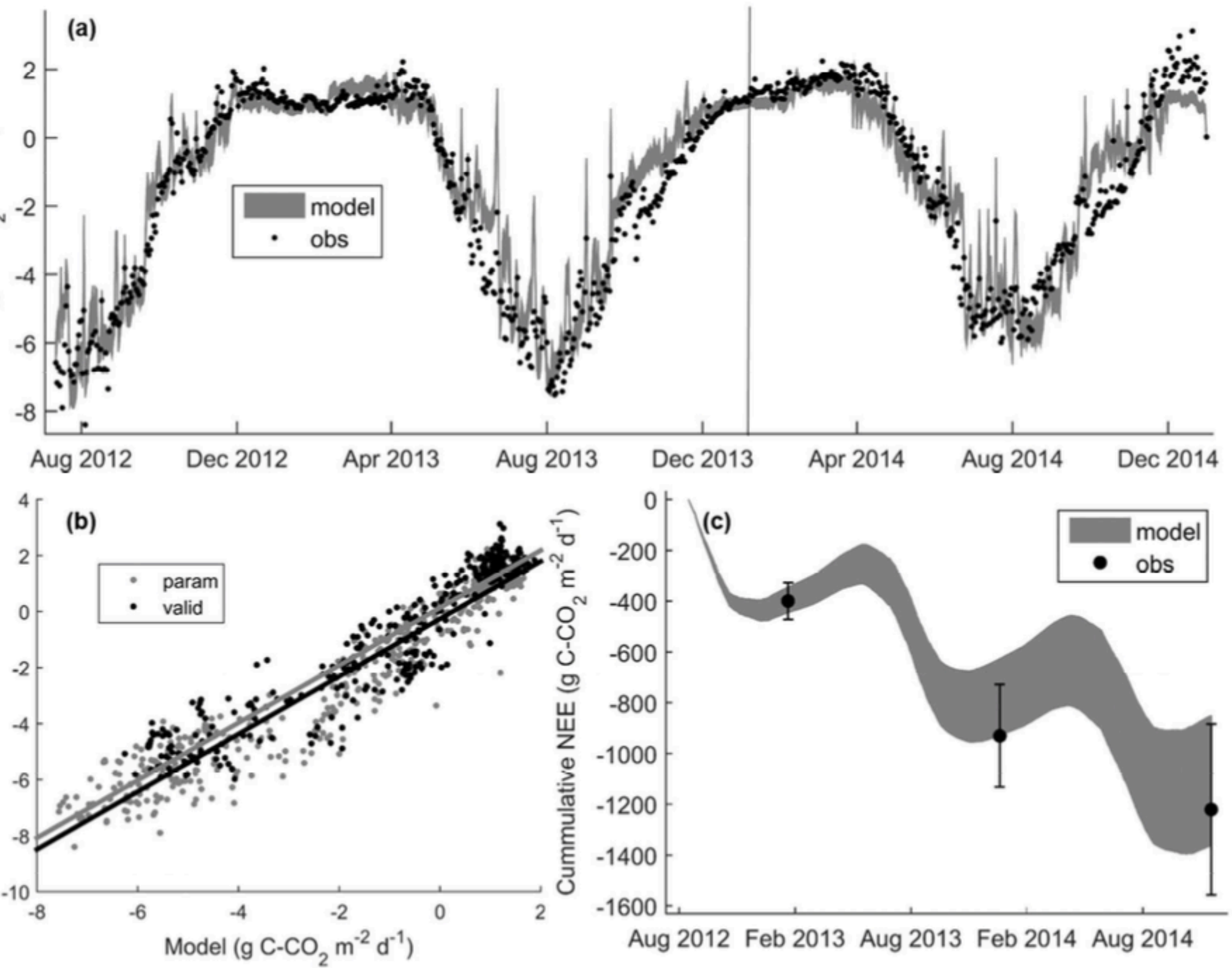
- Search Parameter space with Markov Chain Monte Carlo (MCMC) approach with a delayed rejection adaptive Metropolis-Hastings algorithm

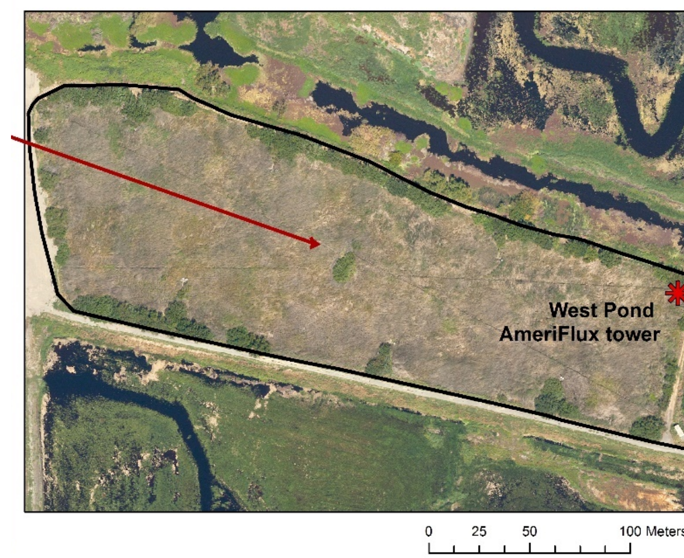
$$J = \sum_{t=1}^{N} \left(\frac{y(t) - p(t)}{\sigma(T)} \right)^2$$

Likelihood Function

obitz, J. M., et al. 2011. A primer for data assimilation with ecological models using Markov Chain Monte Carl
MCMC). Oecologia **167**:599-611.

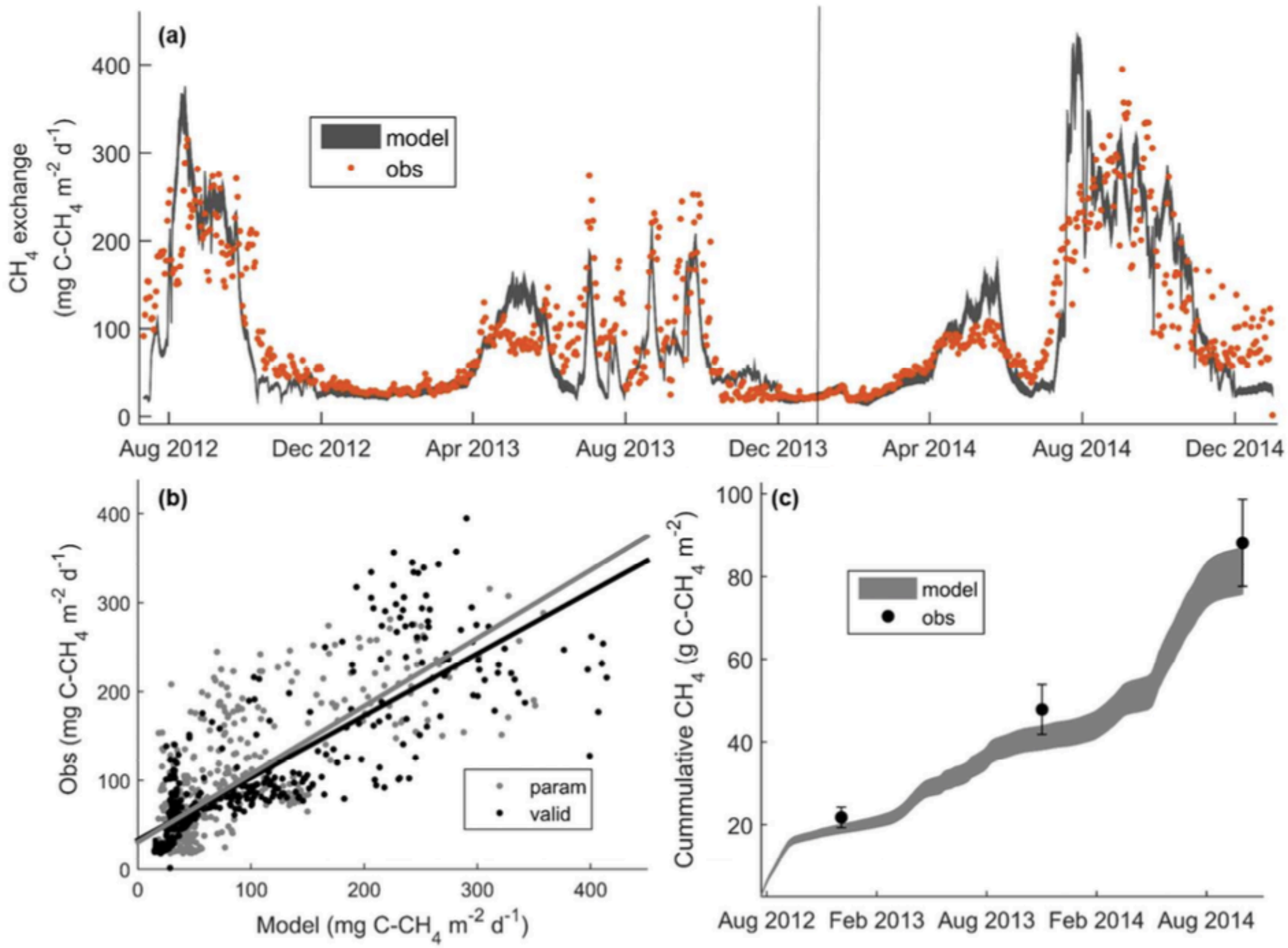
Model Performance:
CO_2 Exchange of Restored Wetland





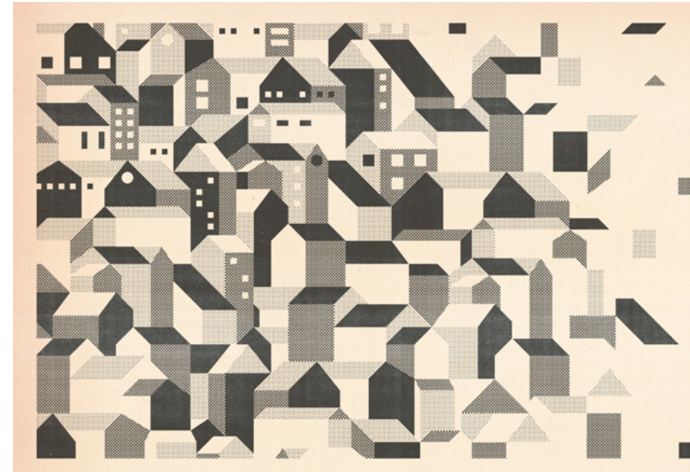
a et al. JGR, to be submitted

Model Performance:
CH_4 Exchange of Restored Wetland



a et al. JGR to be submitted

Deconstructing the Model



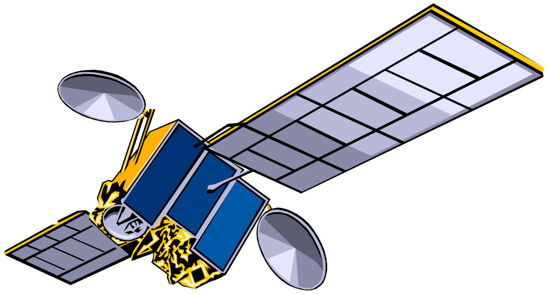
- Model and Measure Photosynthesis
  - How Much Detail in the Model
  - Potential Biases and Errors in Canopy Photosynthesis Measurements
- oil Respiration and Methane Production
  - Roles of Water Table, Photosynthesis and Temperature

http://andrewholder.net/wp-content/uploads/2013/12/deconstruction.jpg

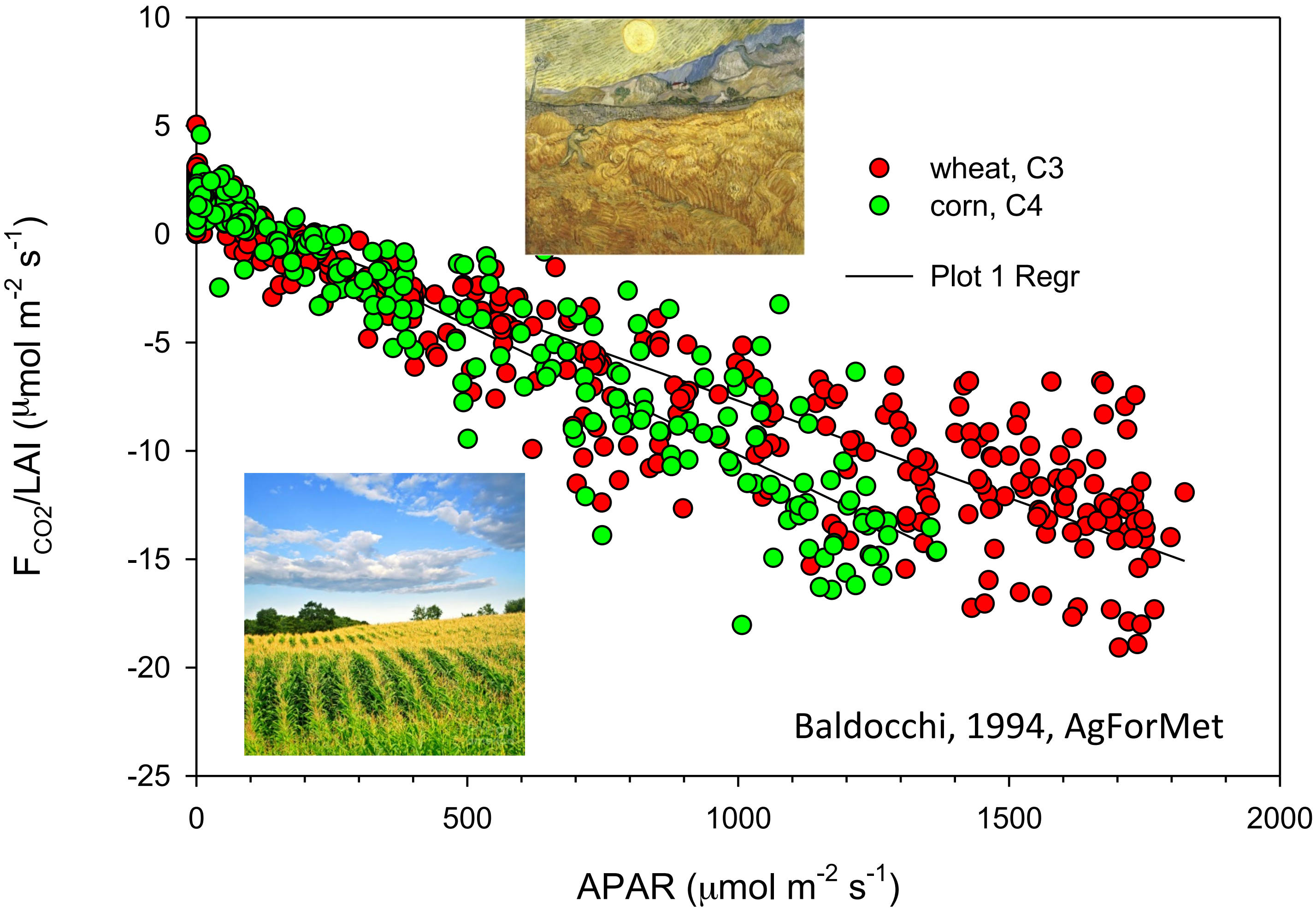
Upscaling Photosynthesis:

Light Use Efficiency and Gross Primary Productivity

$$GPP = LUE * APAR * f(T_k)$$



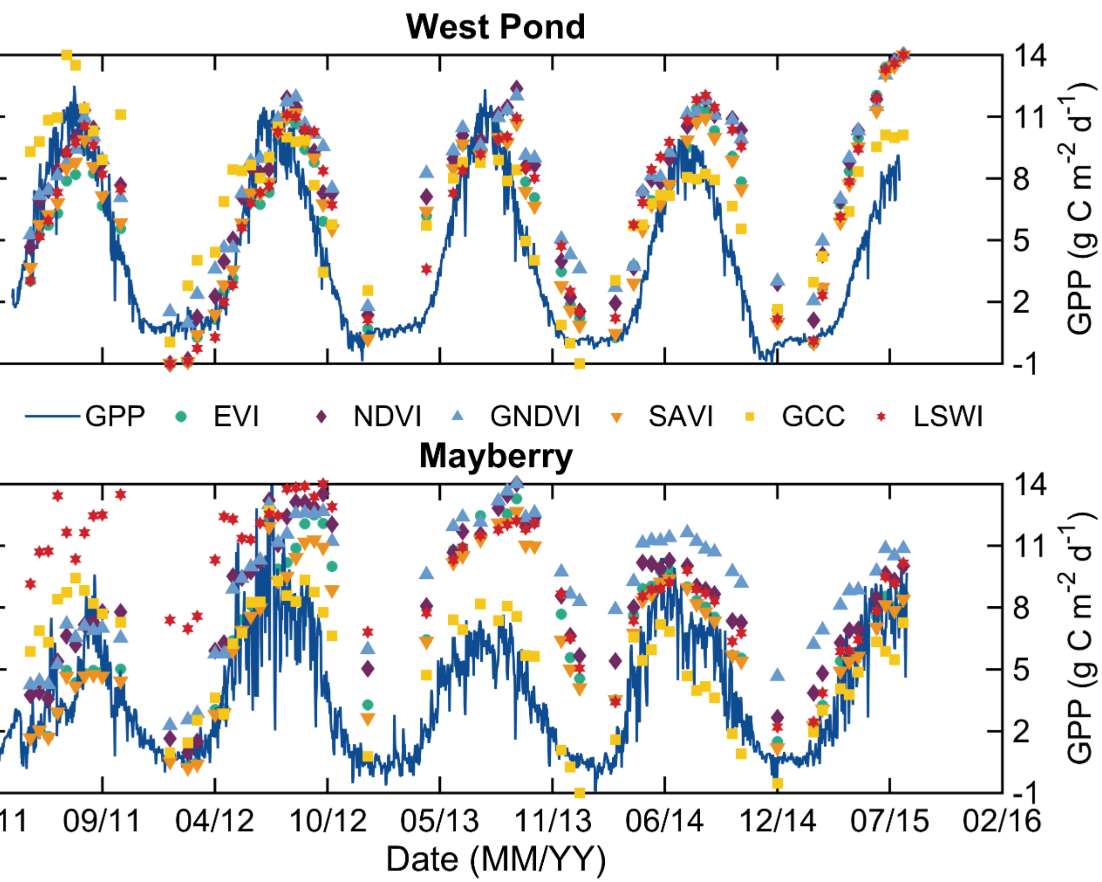
Net Carbon Exchange of Wheat, C_3, and Corn, C_4. Crops with Absorbed Light

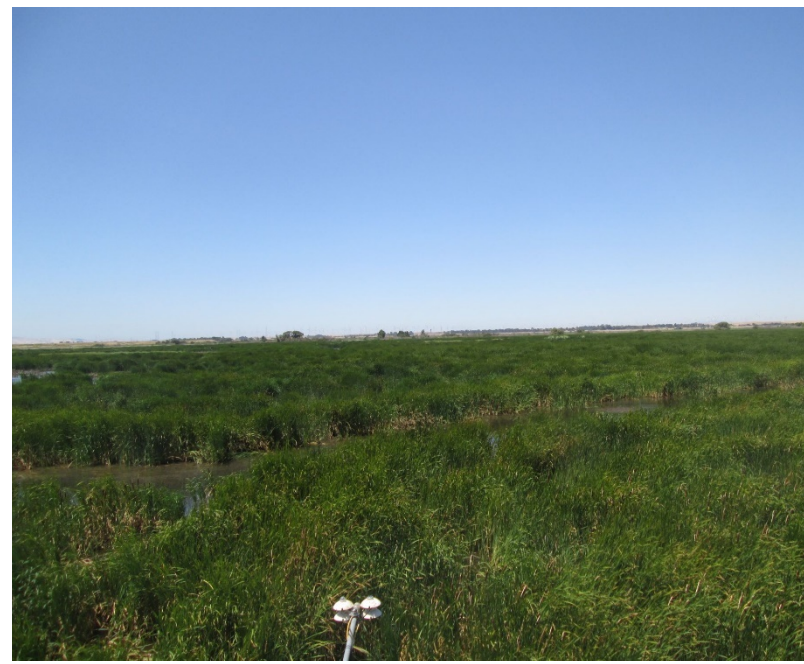


Simple Systems, Light Absorption Explains over 80% of Variance in CO2 Exchange!;
Basis for Satellite Remote Sensing of Global Photosynthesis

Digital Cameras Provide Information on Dynamics of Vegetation Indices

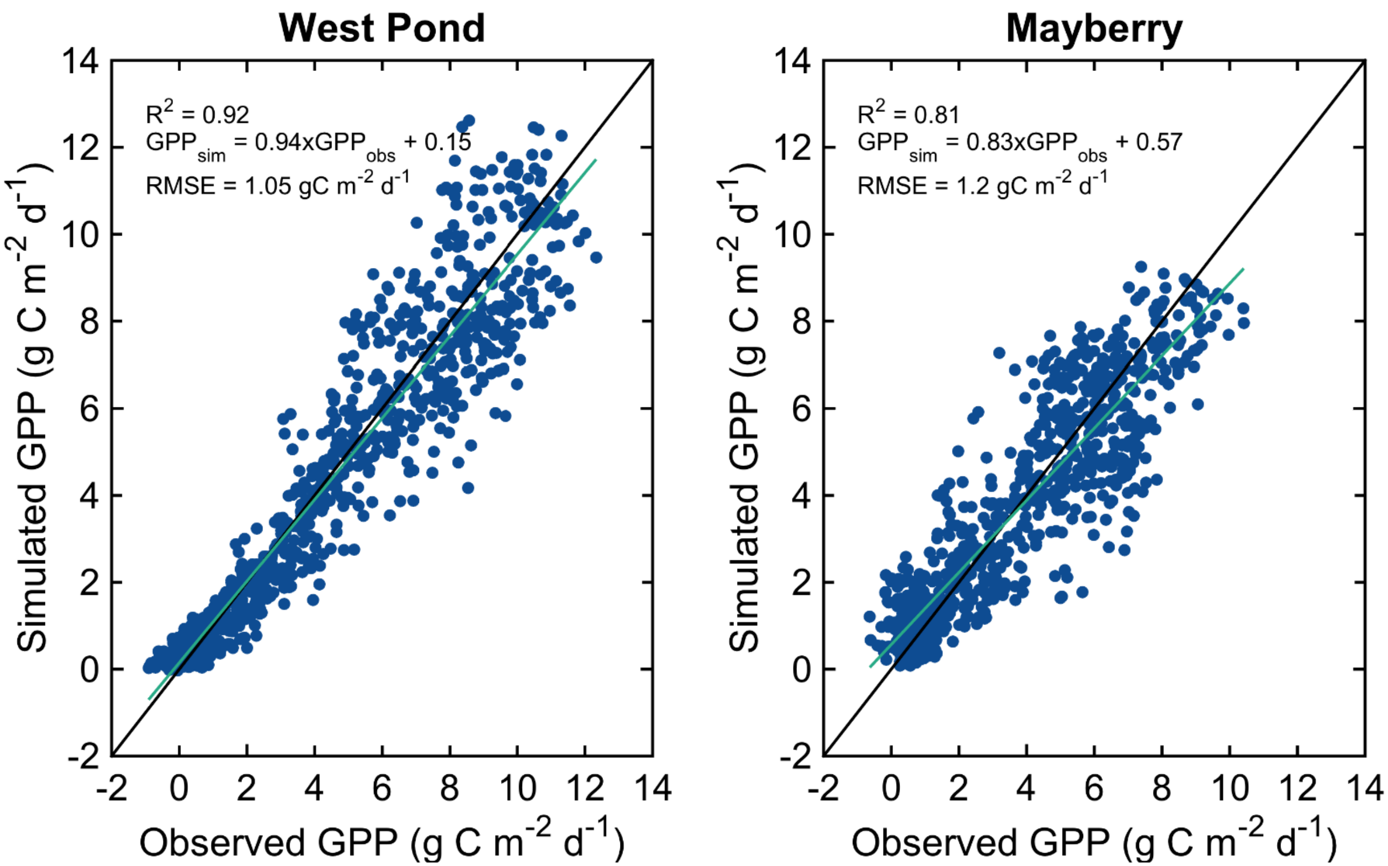
$$FPAR = 0.95(1 - \exp(-k * LAI))$$





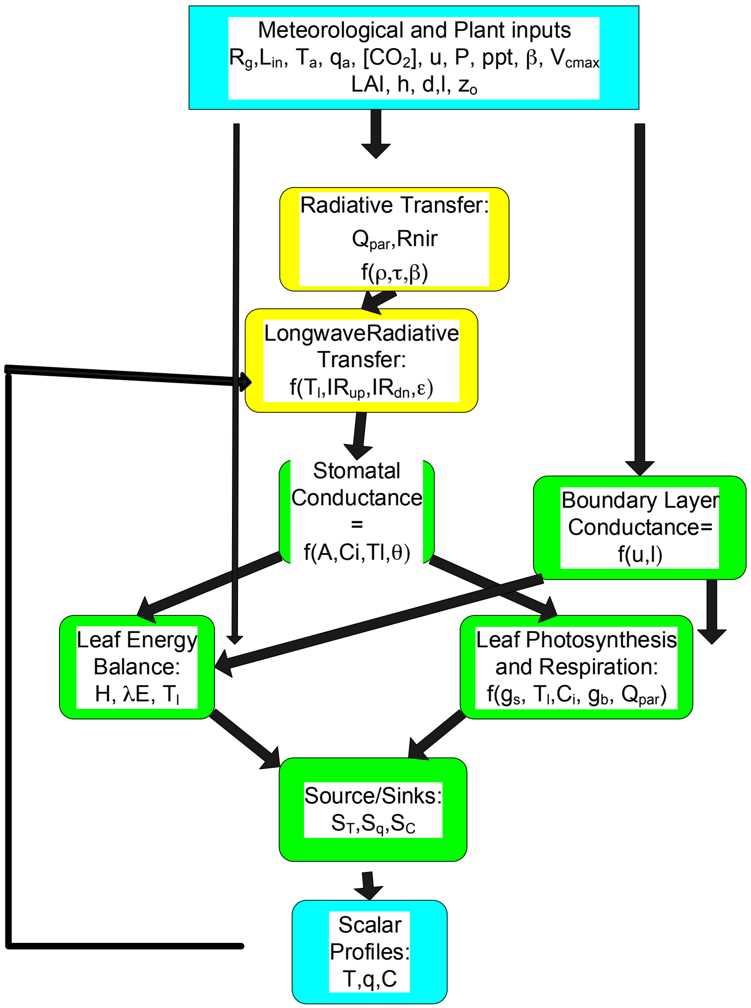
Estimate GPP with Vegetation Index Information from Digital Cameras (RG

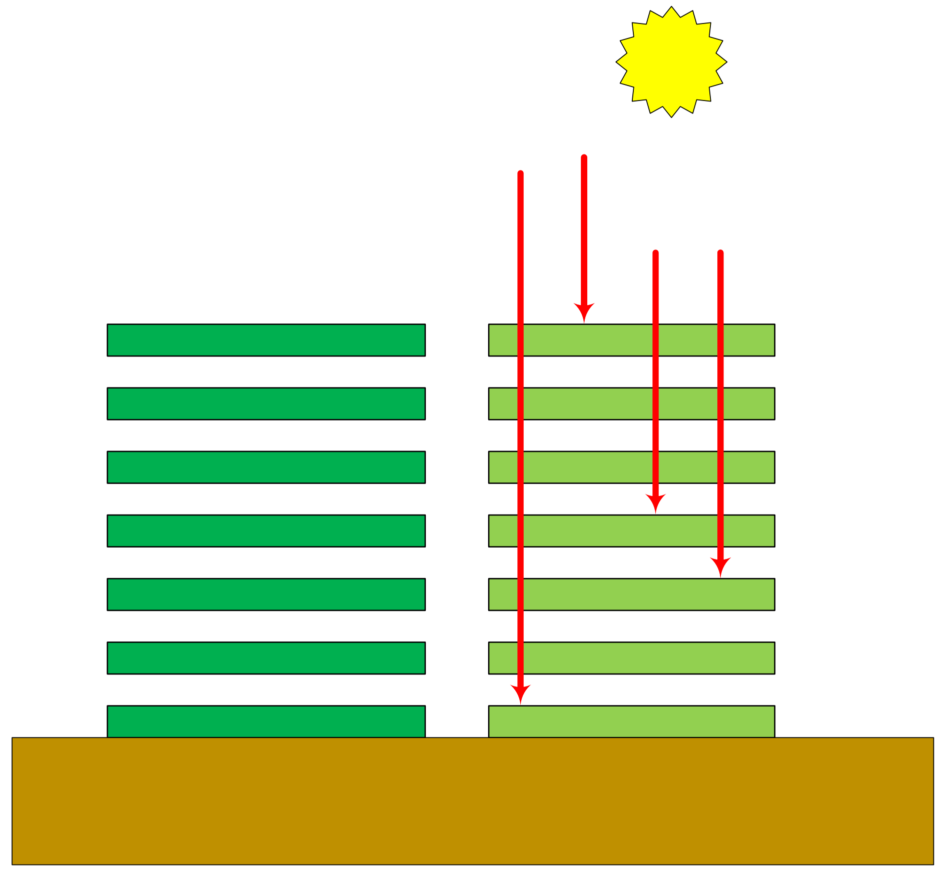
$$GPP = \varepsilon \cdot \left(a_0 + a_1 VI\right) \cdot PAR$$



al. in prep

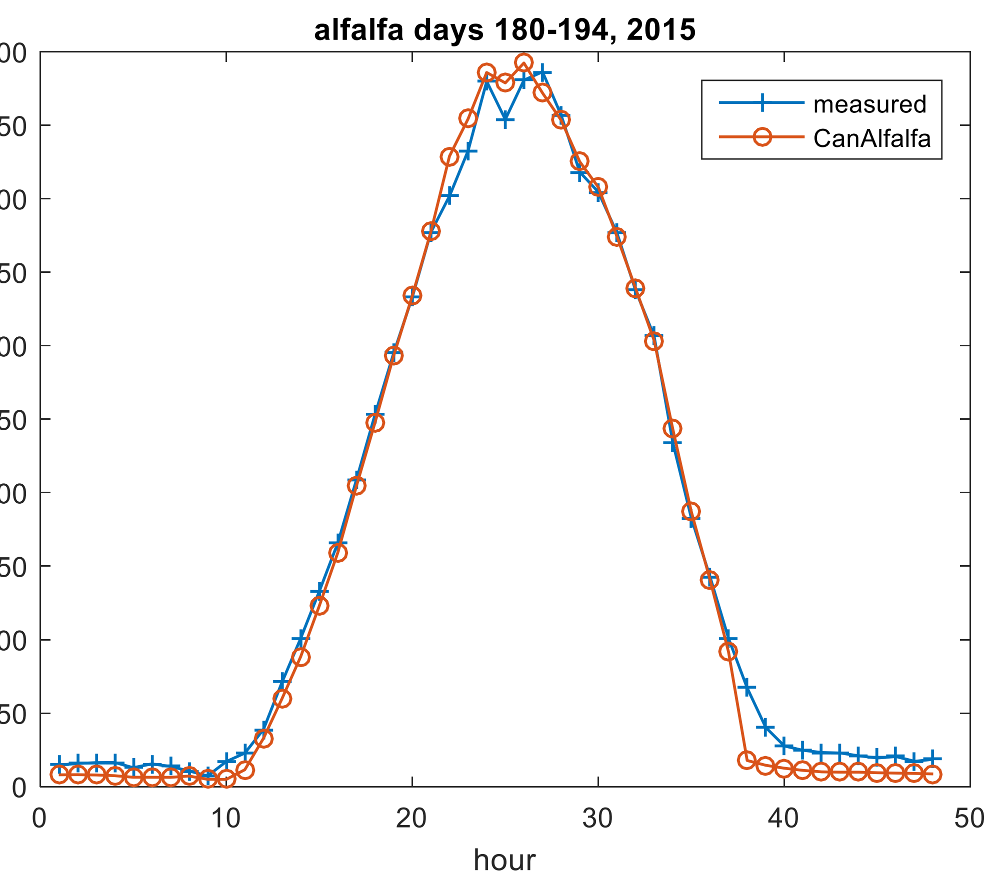
EG, Multi-Layer, coupled photosynthesis-stomatal conductance-energy balance m

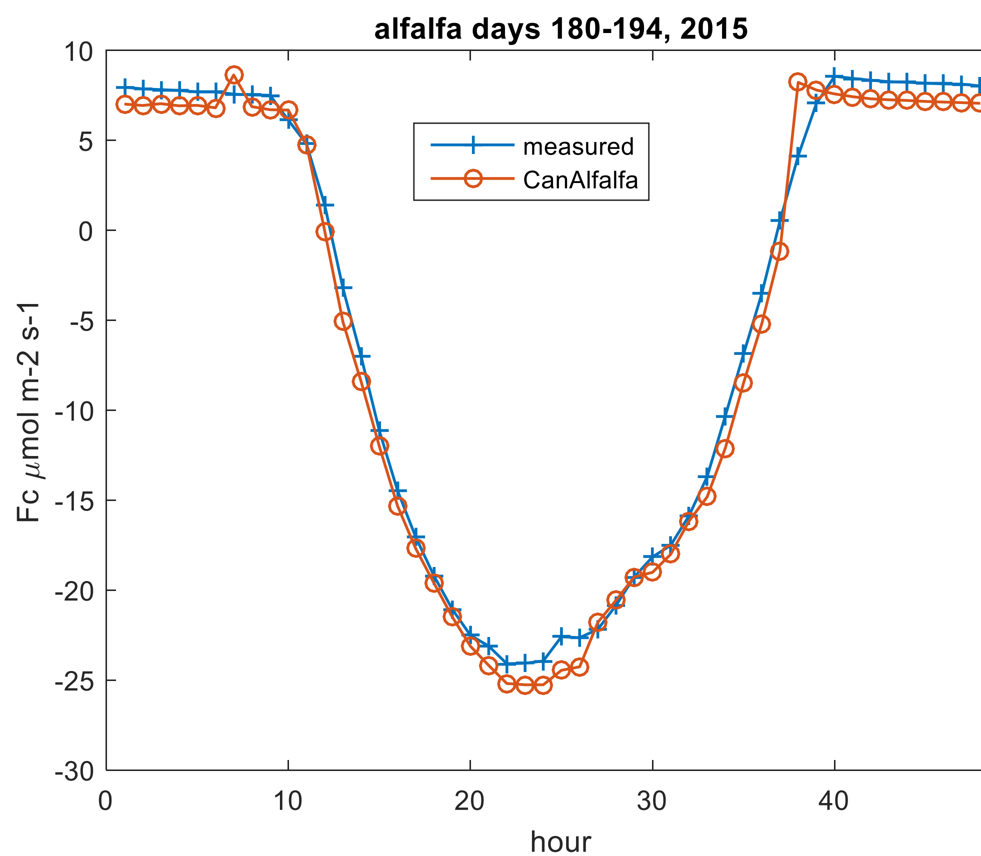




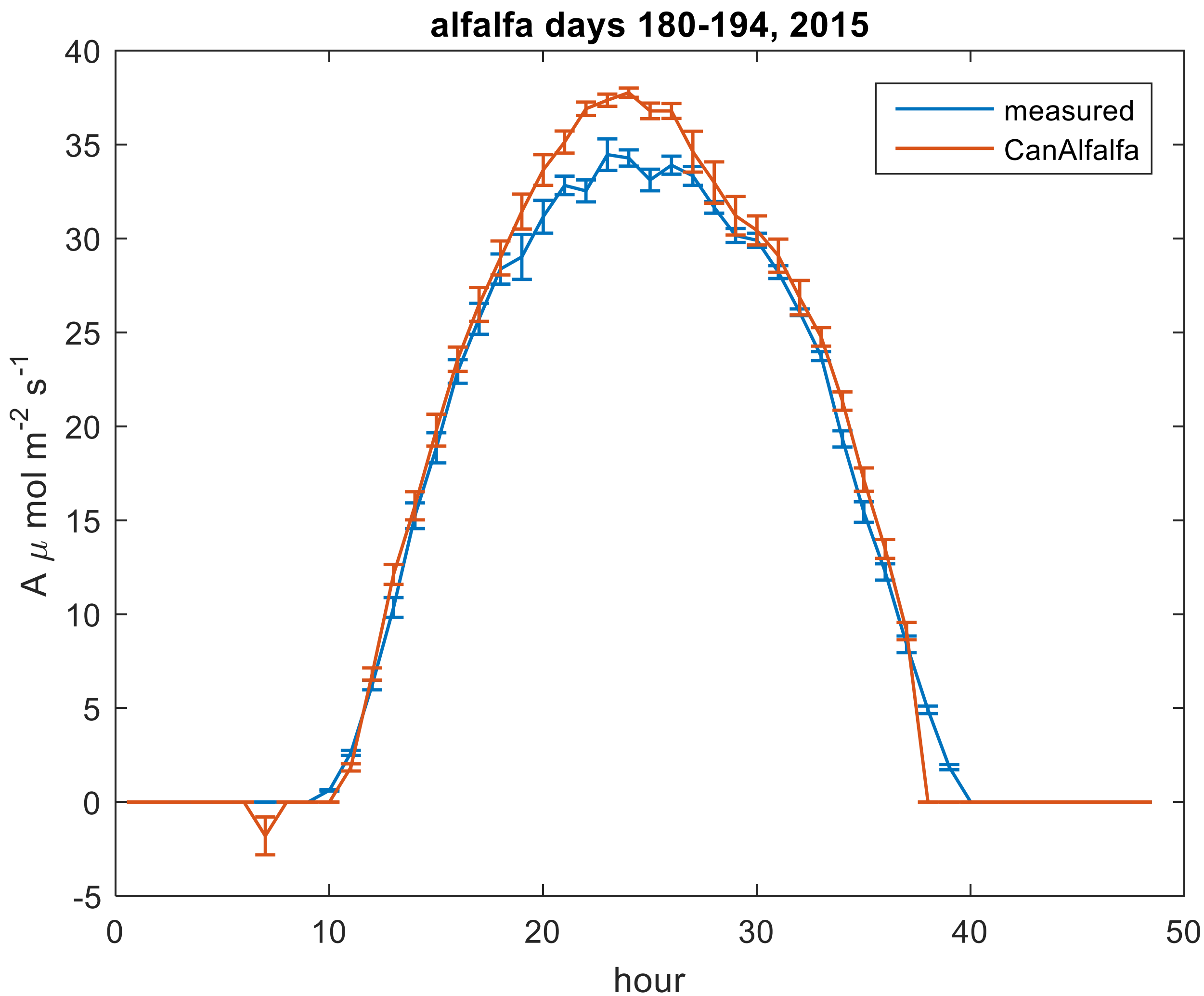
Inputs: Meteorological Conditions, Leaf Area Index, Vcmax;
No Tuning!

Latent Heat and Net Ecosystem Carbon Exchange

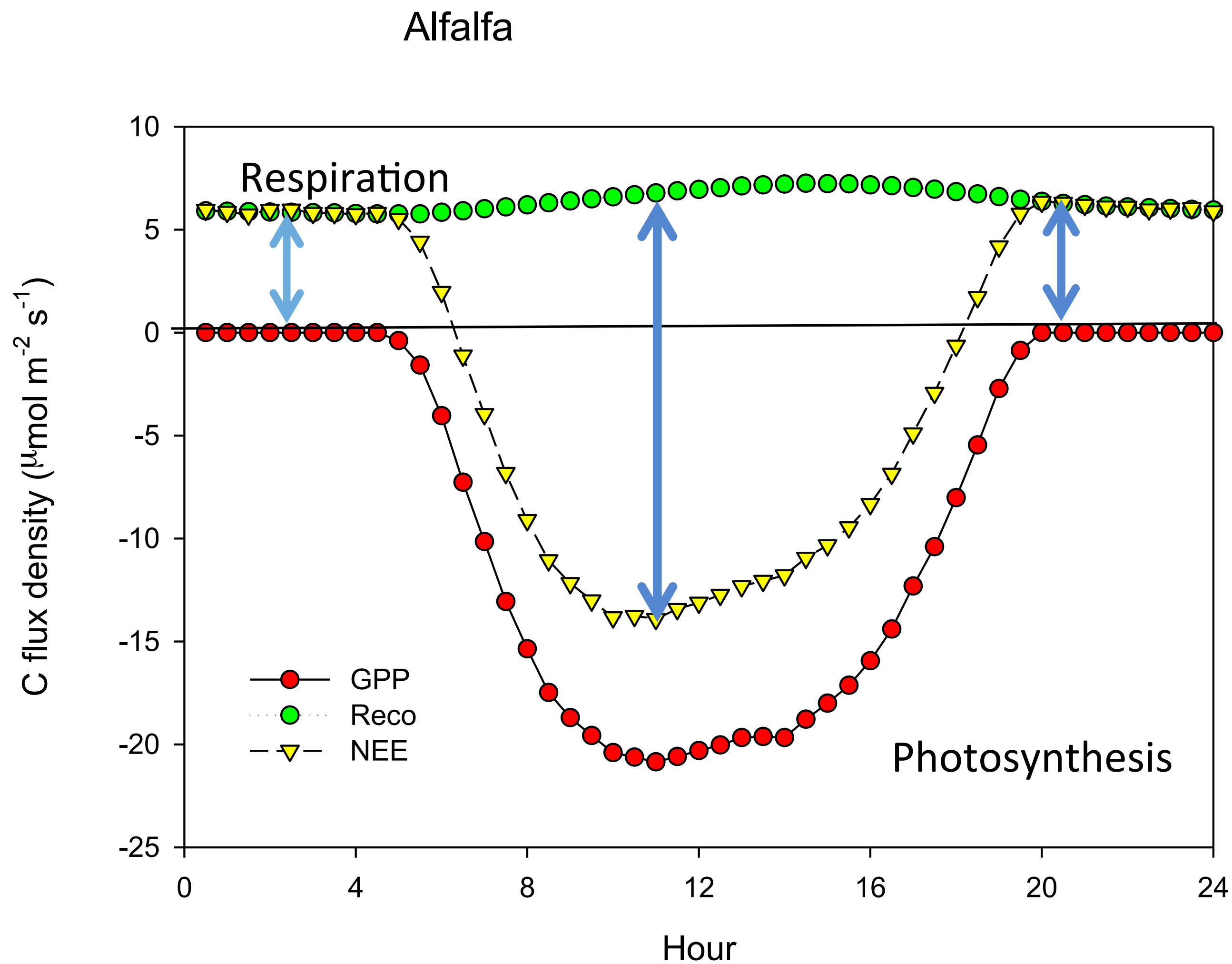




Canopy Photosynthesis, A, given Meteorology, LAI and V_{cmax}



Do We Trust Canopy Photosynthesis Test Data?



Can We Extrapolate Ni
Respiration to Day as
Function of Temperatu

Is Dark Respiration
Inhibited in Light due t
Kok Effect?

Deduce Photosynthesis and Respiration from Diel Course of NEE

Baldocchi and Sturtevant, 2015, AgForMet

An Artifact of Spurious Correlation Among NEE, GPP and R_{eco}?

Closure Problem of One Equation and Two Unknowns

$$NEE = GPP + Reco$$

Correlation using Day/Night Sampling

$$G = NEE_{day} - R_{eco,day} = x - z$$

$$R = NEE_{night} + R_{eco,day} = y + z$$

Self correlation

$$r_{sc} = \frac{-\overline{z'z'}}{(\overline{x'x'} + \overline{z'z'})^{1/2}(\overline{y'y'} + \overline{z'z'})^{1/2}}$$

r_{sc} = -0.157

alfalfa

Baldocchi and Sturtevant, 2015 AgForMet

System of Equations with New and Independent Information from ^{13}C

$$NEE = GPP + Reco$$

Bowling Method

Fluxes of the stable isotope $^{13}CO_2$

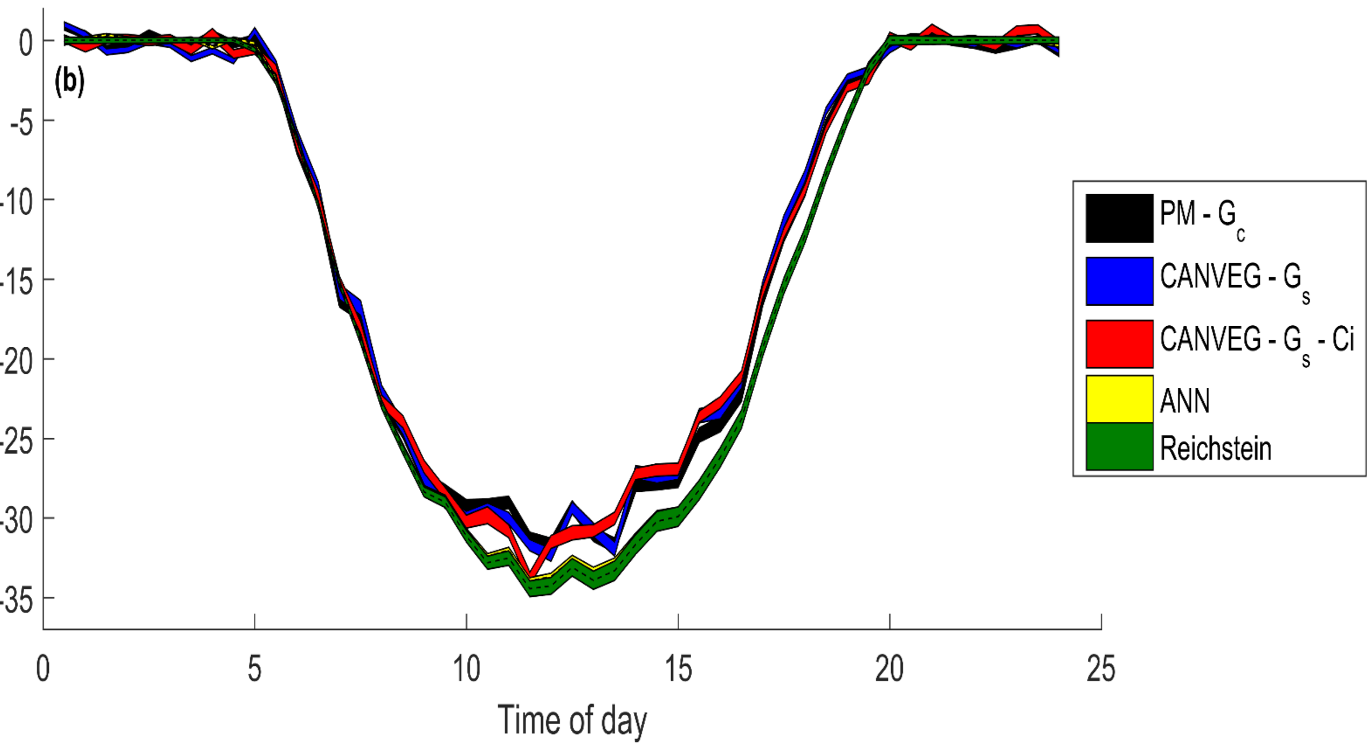
$$isoflux = \delta^{13}C_r \cdot R_{eco} + (\delta^{13}C_a - \Delta) \cdot GPP$$

Eddy covariance (1 Hz) with closed path CO2 isotope analyze
CCIA-48 Los Gatos Research

Mid infrared quantum cascade laser with high precision

$\delta^{13}C$: 0.7 per mill, $^{13}CO_2$: 2 ppb

Tests of Three Ways to Partition NEE into GPP: Methods ~ are Intercomparable



Method	GPP cumulative (g CO_2-C m^{-2})
Isotope	-190 ± 5
ANN	-210 ± 4
Reichstein	-213 ± 5

Oikawa et al. in prep for Ag. Forest M

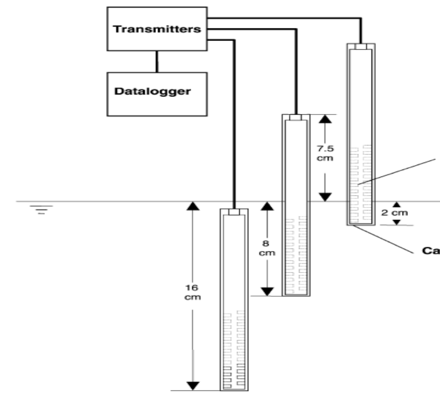
Alfalfa, Summer, 2015

ntinuous Soil Respiration

- Continuous Soil CO2 Efflux Measurement Systems

  - Profile method (n=2)

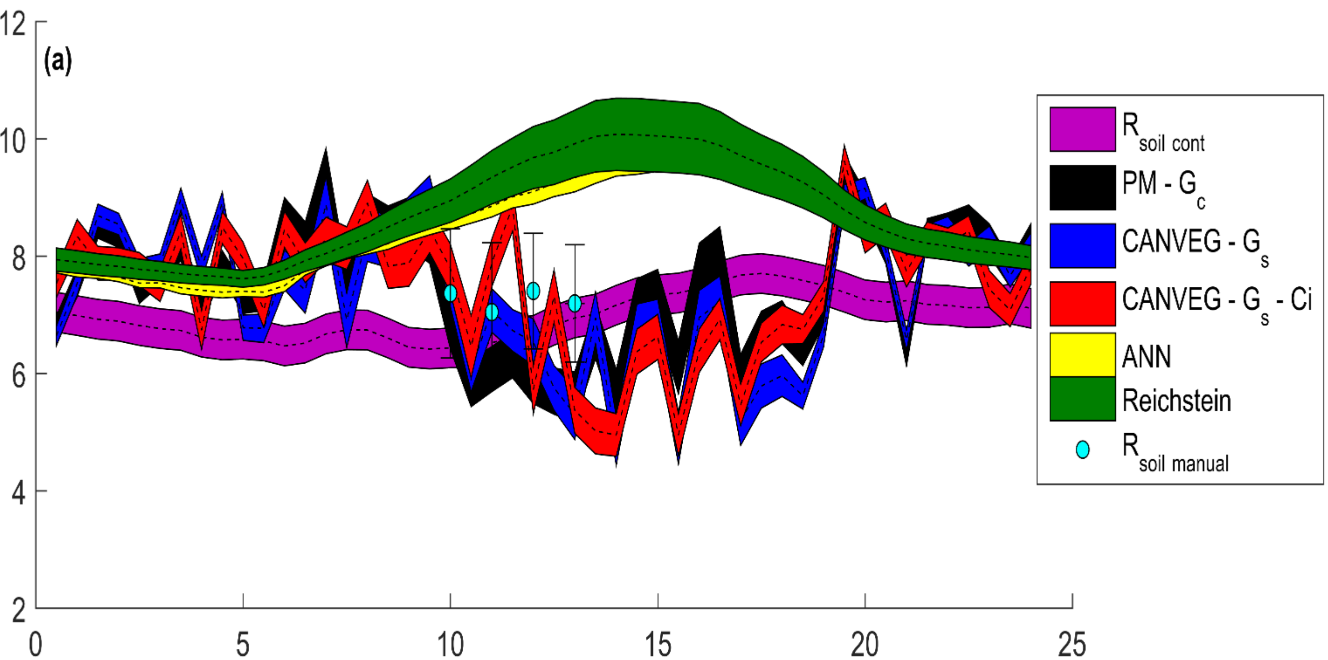
$$R_{soil} = -D_s \frac{dC}{dz}$$



  - Forced diffusion chamber (n=1)

$$R_{soil} = G_{diff}(C_{chamb} - C_{atm})$$

Measured and Modeled CO2 Efflux Data are Intercomparable

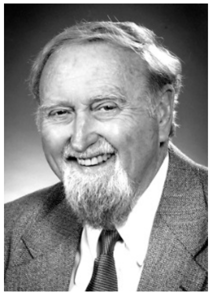


Method	R_{eco} cumulative (g CO_2-C m^{-2})
Isotope	115 ± 5
ANN	132 ± 3
Reichstein	135 ± 5
R_{soil}	108 ± 5

Oikawa et al. in prep for Ag. Forest Met.

New Math to Look at Cause and Effect

- Artificial Neural Networks
- Granger Causality
- Transfer Entropy
- Shannon Entropy
- Mutual Information Theory



Artificial Neural Networks

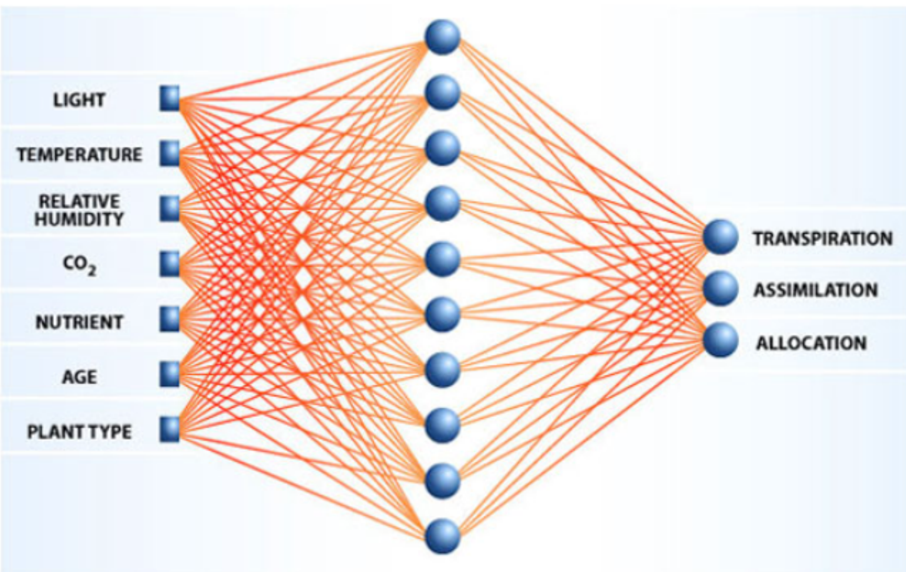
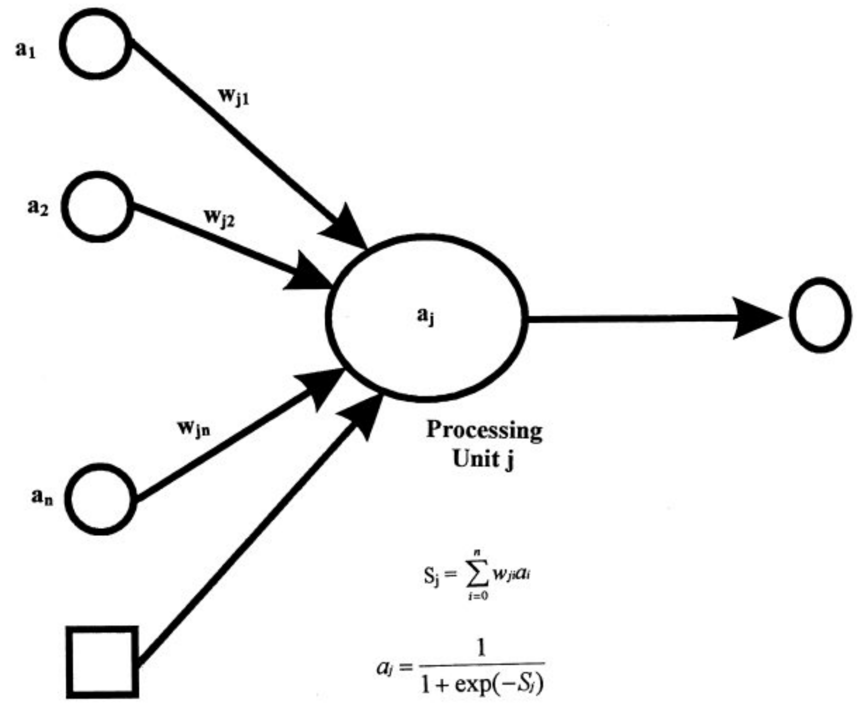


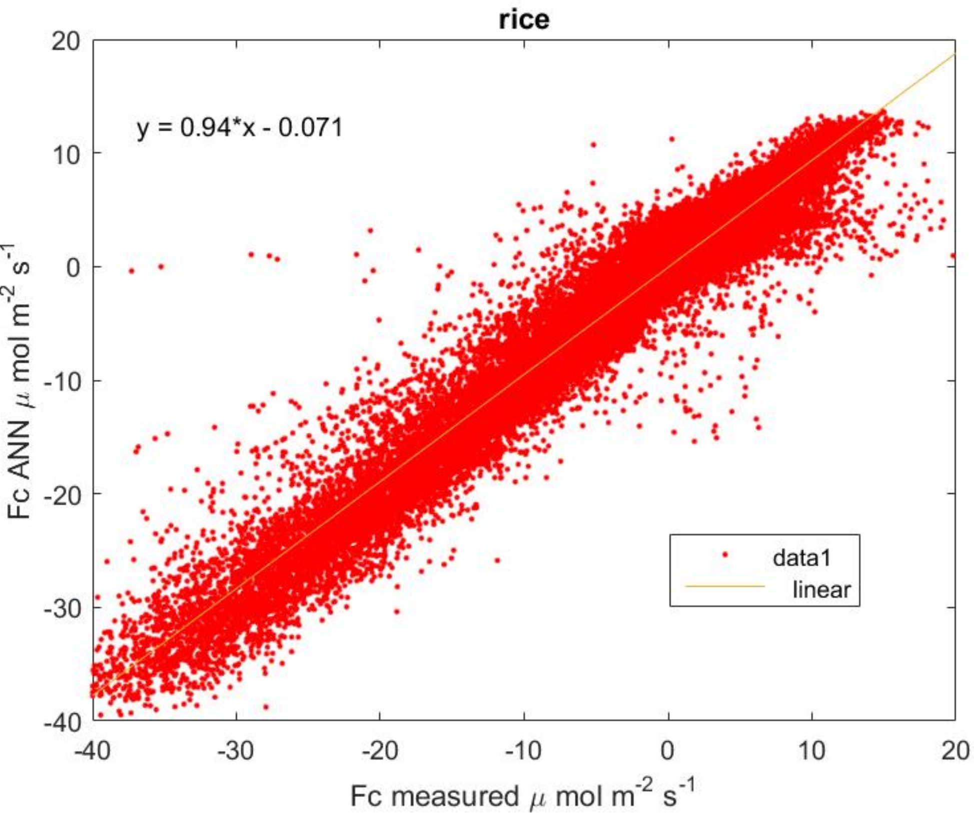
Fig.1 Layer Structure of Neurons and their connections[1]



http://media.developeriq.in/images/neurons1.png

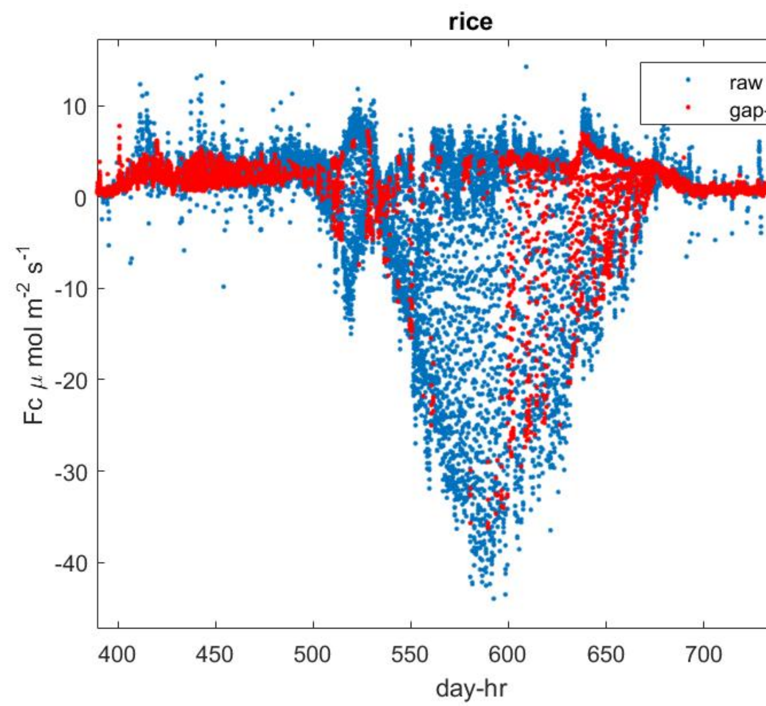
Cancer
Volume 91, Issue S8, pages 1615-1635, 17 APR 2001 DOI: 10.1002/1097-0142(20010415)91:8+<1615::AID CNCR1175>3.0.CO;2-L
http://onlinelibrary.wiley.com/doi/10.1002/1097-0142(20010415)91:8%2B<1615::AID-CNCR1175>3.0.CO

Neural Network CO2 Fluxes (Fc) vs Measurements



Inputs:

TA
PAR
VPD
WT_gf
ustar
Mdate



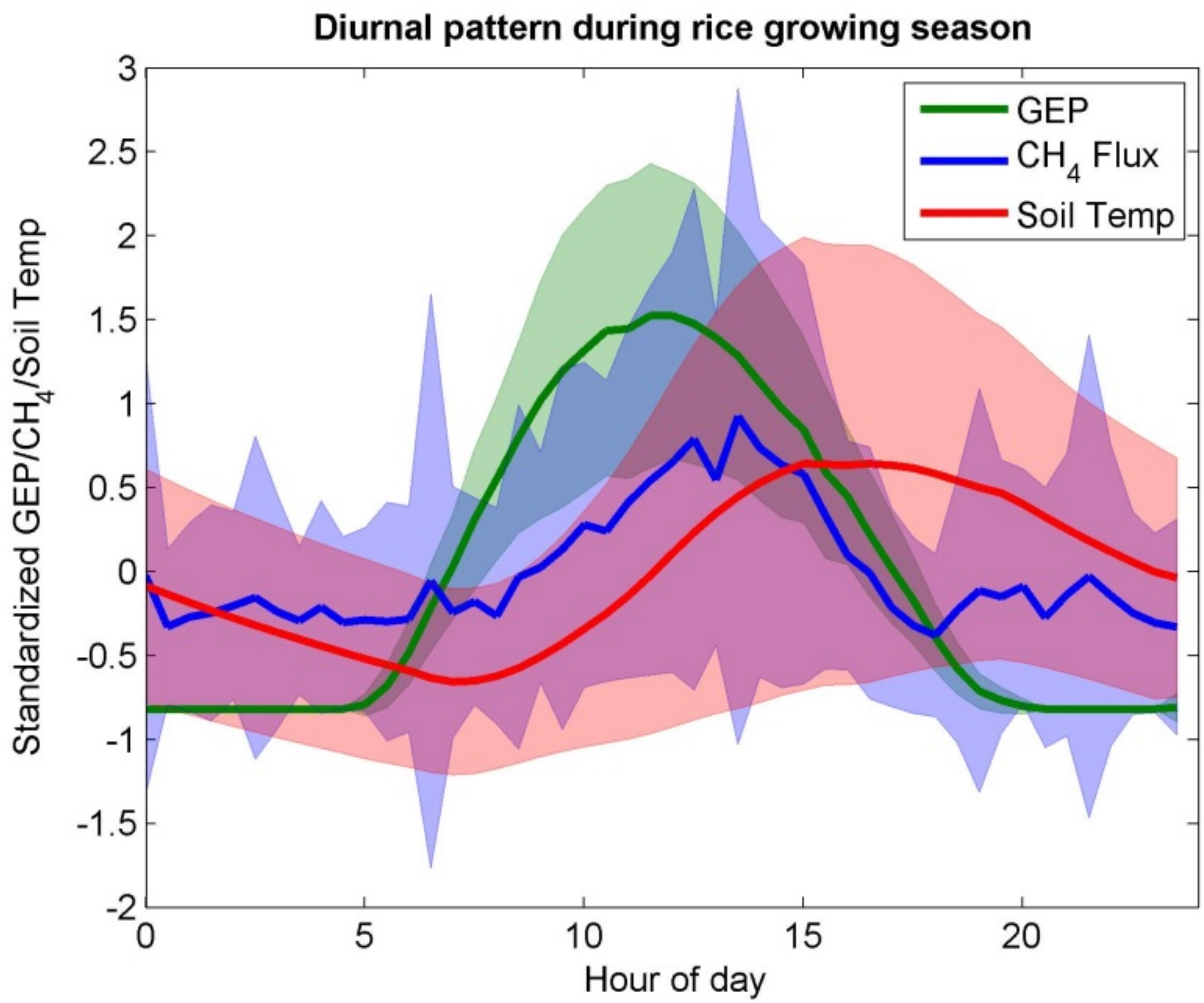
Biophysical Controls on Methane Fluxes

		Pairwise	Stepwise Linear		Neural Network	
		r^2	r^2	AIC	r^2	AIC
wing season						
9-2015	GEP	0.622	0.386	2853	0.258	7704
	WTD	0.575	0.424	2793	0.462	7431
	ER	0.168	0.458	2737	0.713	6853
	LE	0.452	0.469	2718	0.751	6716
	u_*	0.147	0.470	2718	0.765	6671
	T_a	0.309	0.471	2717	0.814	6462
	T_s	0.195	0.474	2712	0.825	6420

Neural Network Expl
of variance in Me
Fluxes

Knox et al in press JGR Biogeos

Photosynthesis Primes Methane Production in Rice, which Leads Temperature



Hatala et al. GRL 2012

Granger causality:
A measure of coupling with explicit time directionality

Compare the bivariate model:

$$x_n = \sum_{j=1}^{m} a_{1,j} x_{n-j} + \sum_{j=1}^{m} a_{2,j} y_{n-j} + \varepsilon_n,$$

To the univariate case:

$$x_n = \sum_{j=1}^{m} a_j x_{n-j} + \eta_n$$

Calculate G-causality:

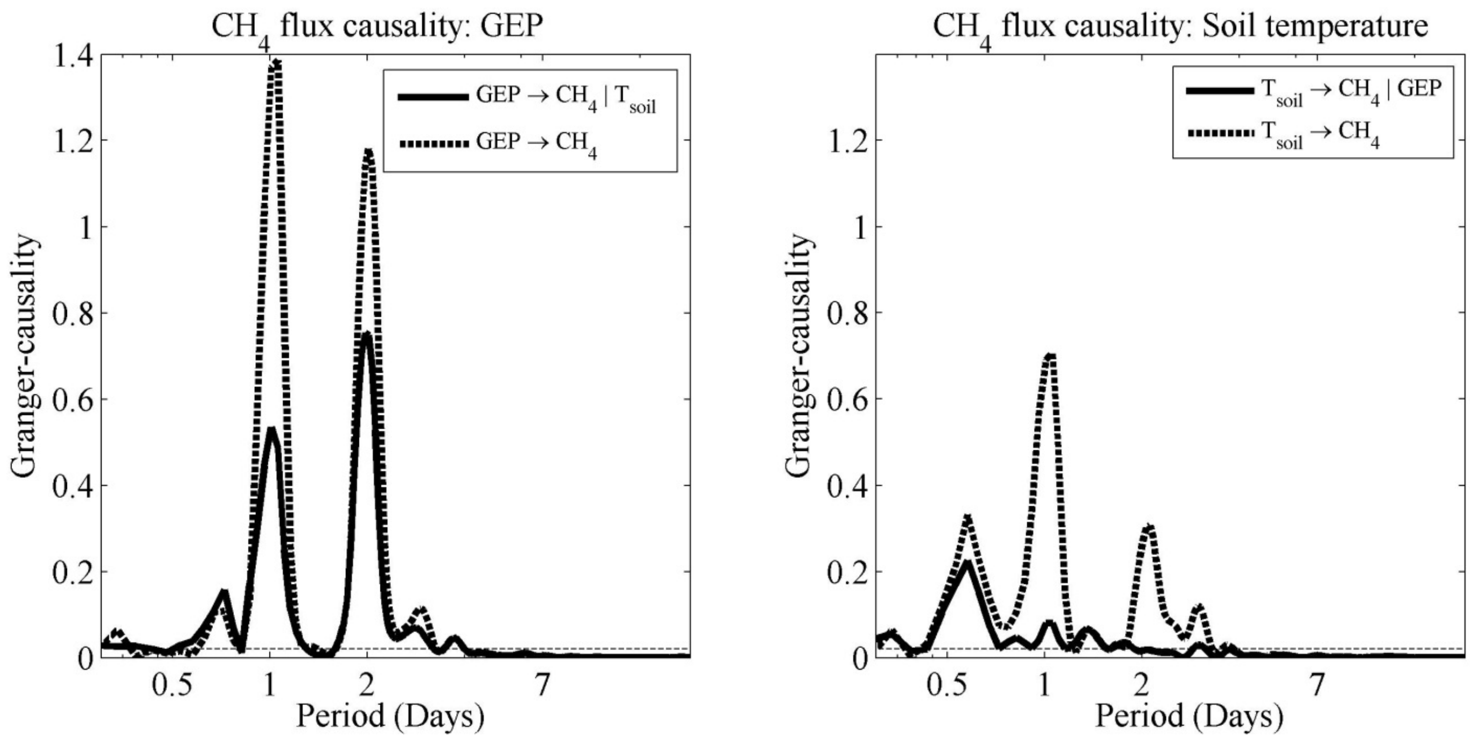
$$G_{y \to x} = \ln \frac{\sigma_\eta^2}{\sigma_\varepsilon^2}$$

No interaction, G ≈ 0
Interaction, G > 0

A variable, x, Granger Causes
y if the bivariate equation outperforms
The univariate

Detto et. al., *Am. Nat.* [2012]
Geweke, *JASA* [1982]
Dhamala, *Phys. Rev. Lett.* [2008]
Chen, *J. Neurosci. Meth.* [2006]

Methane scales with Photosynthesis, better than Temperature



Hatala et al. GRL 2012

Mutual Information

$$I_{XY} \underset{(9)}{=} \sum_{x_t}\sum_{y_t} p(x_t, y_t)\log_2 \frac{p(x_t, y_t)}{p(x_t)p(y_t)}$$

$$I_{XY} = H_X + H_Y - H_{XY}$$

Relative Mutual Information

$$I_{XY}^R = I_{XY} / H_Y$$

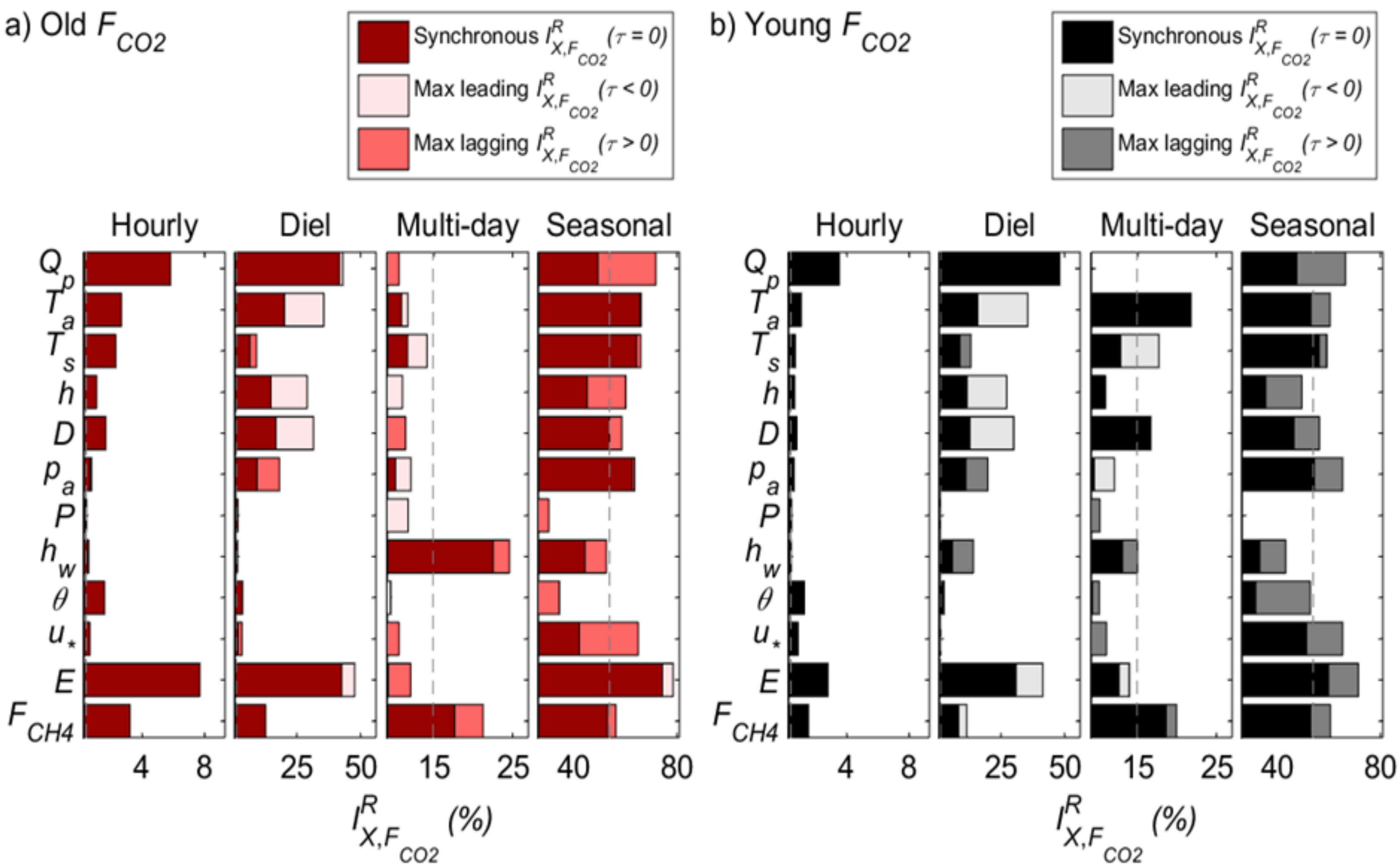
Shannon Entropy

$$H_X = -\sum_{x_t} p(x_t)\log_2 p(x_t)$$

$$H_{XY} = -\sum_{x_t}\sum_{y_t} p(x_t, y_t)\log_2 p(x_t, y_t)$$

$$H_Y = -\sum_{y_t} p(y_t)\log_2 p(y_t)$$

Relative Information on CO_2 Flux



Sturtevant et al. 2016 JGR Biogeoscience

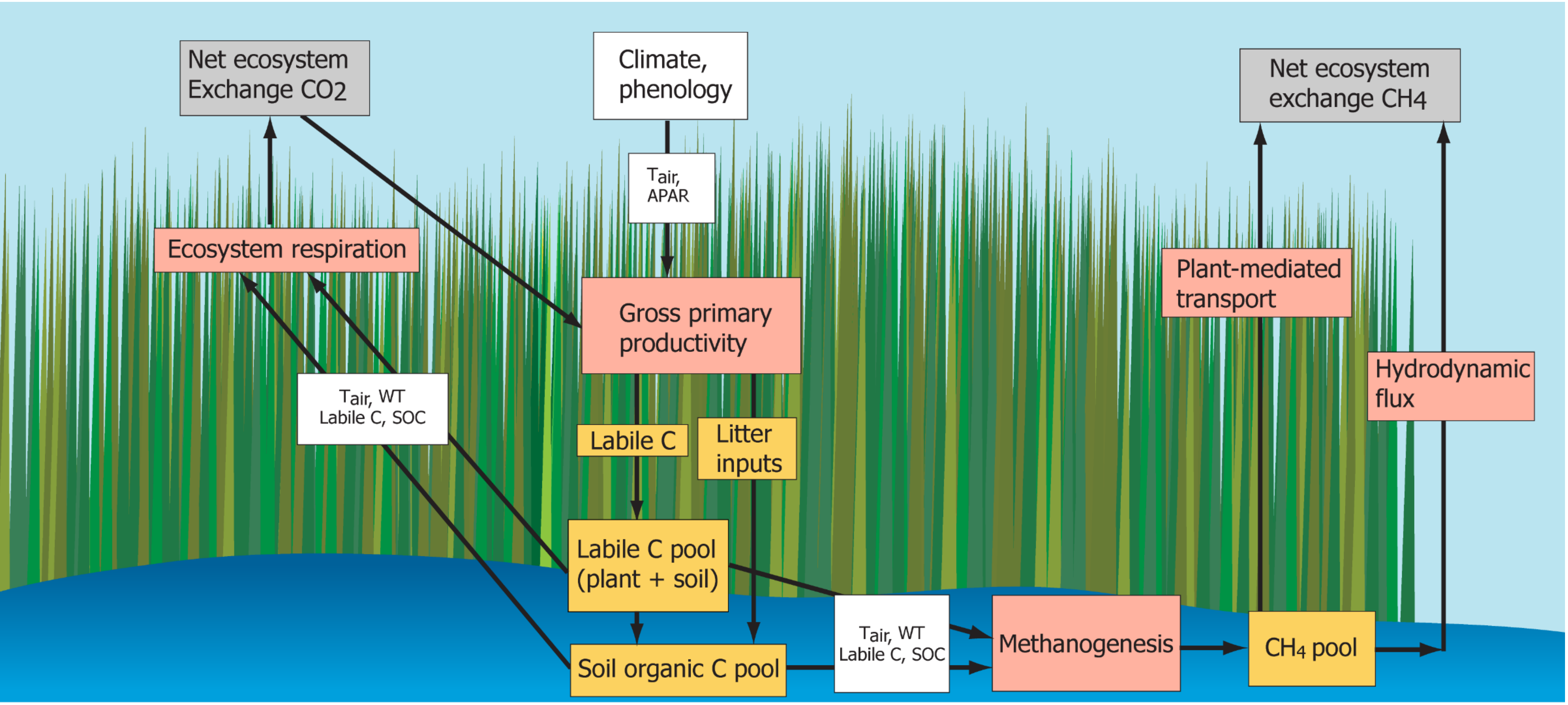
Summary

- With a Suite of Models and Mathematical Tools We Can Deduce the Roles of Biophysical Drivers on Greenhouse Gas Fluxes across as Spectrum of Time Scales
- Simple Models have Potential for Being Used to Inform on Net Carbon Balances for Cap and Trade Markets based on Simple Inputs like Meteorological Conditions and Canopy Greeness
- Tests of Canopy Photosynthesis Measurements based on CanVeg Model, Stable Isotopes and Continuous Soil Respiration Measurements Increase our Confidence on Flux Partitioning Methods at these Sites

Over Arching Ideas

- You Gotta' Get Photosynthesis Right if You Want to Simulate the Dynamics Rest of the C-Related Pools, Processes and Fluxes
- Soil Trace Fluxes (CO2 and Methane) are Tied to Recent Photosynthesis
  - Old paradigm was simple functions dependent upon soil temperature, soil moisture and water table
- Tying a Methane Emission Model to a Simple Photosynthesis model has Merit
- Validating Canopy Photosynthesis Model depends upon how well we can extract information on GPP from NEE
  - New Statistical Model shows Spurious Correlation is Small
  - New Stable Isotope Flux Measurements confirm Validity of Standard Flux Partitioning

RMT: Peatland Ecosystem Photosynthesis, Respiration, and thane Transport Model



RMT Model

Model-data fusion

Markov Chain Monte Carlo (MCMC) approach with adaptive Metropolis-Hastings algorithm

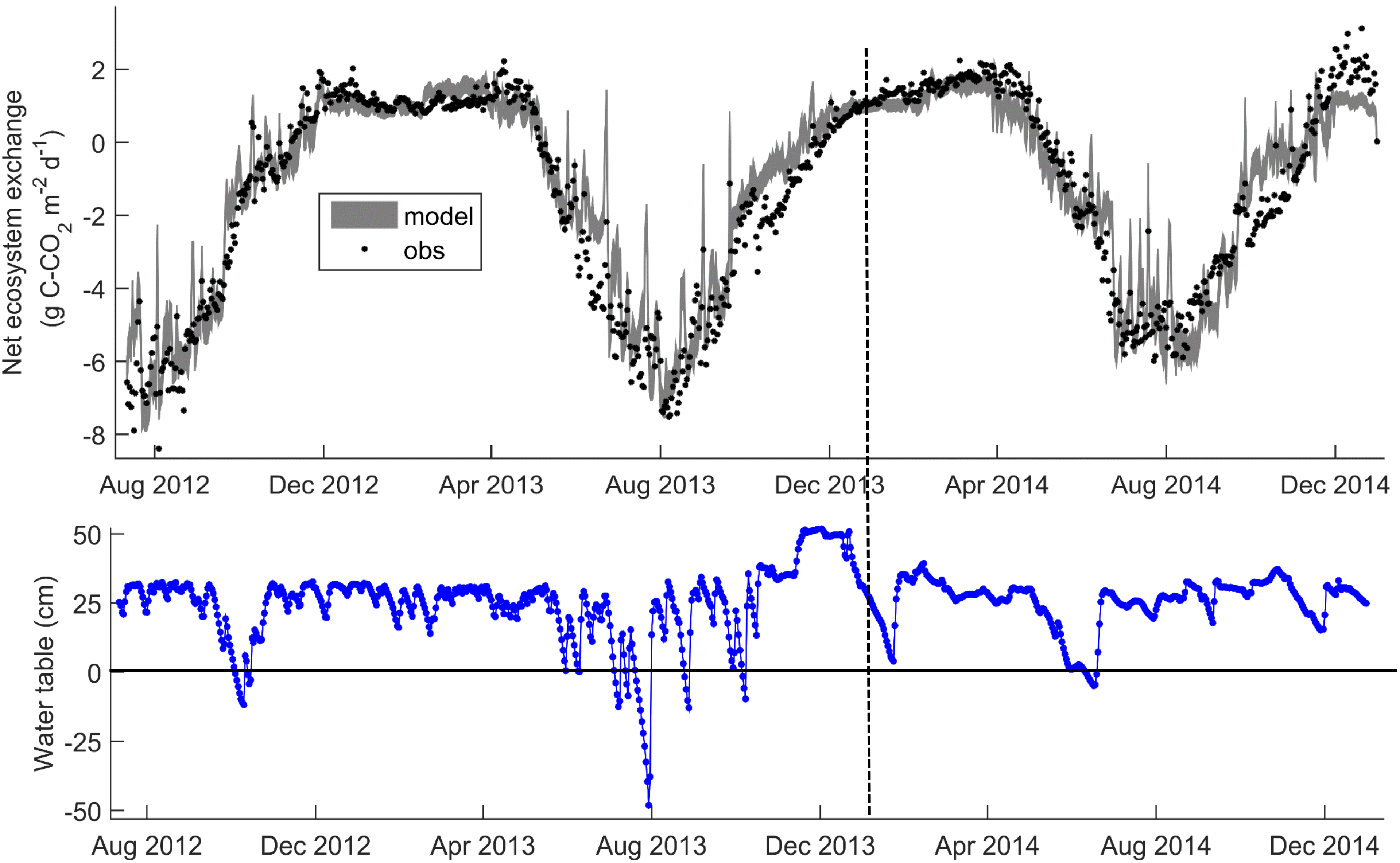
$$J = \sum_{t=1}^{N} \left(\frac{y(t) - p(t)}{\sigma(T)} \right)^2$$

J = data-model mismatch

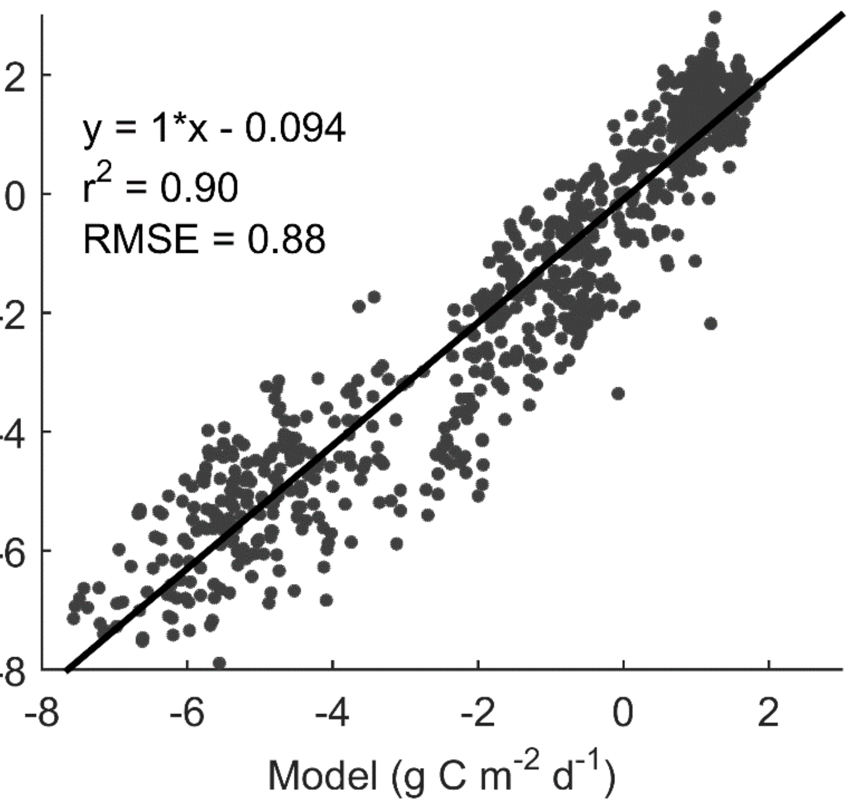
y = observed flux

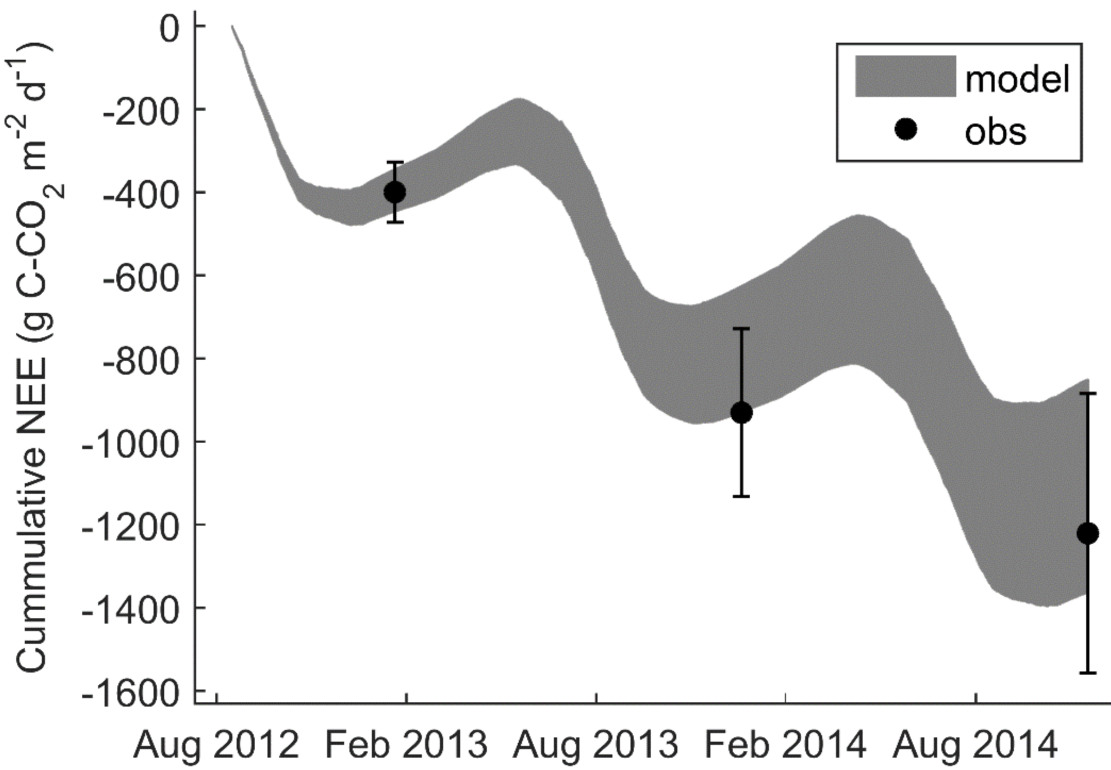
p = modeled flux

σ = uncertainty in the observed flux (gap-filling + random error)



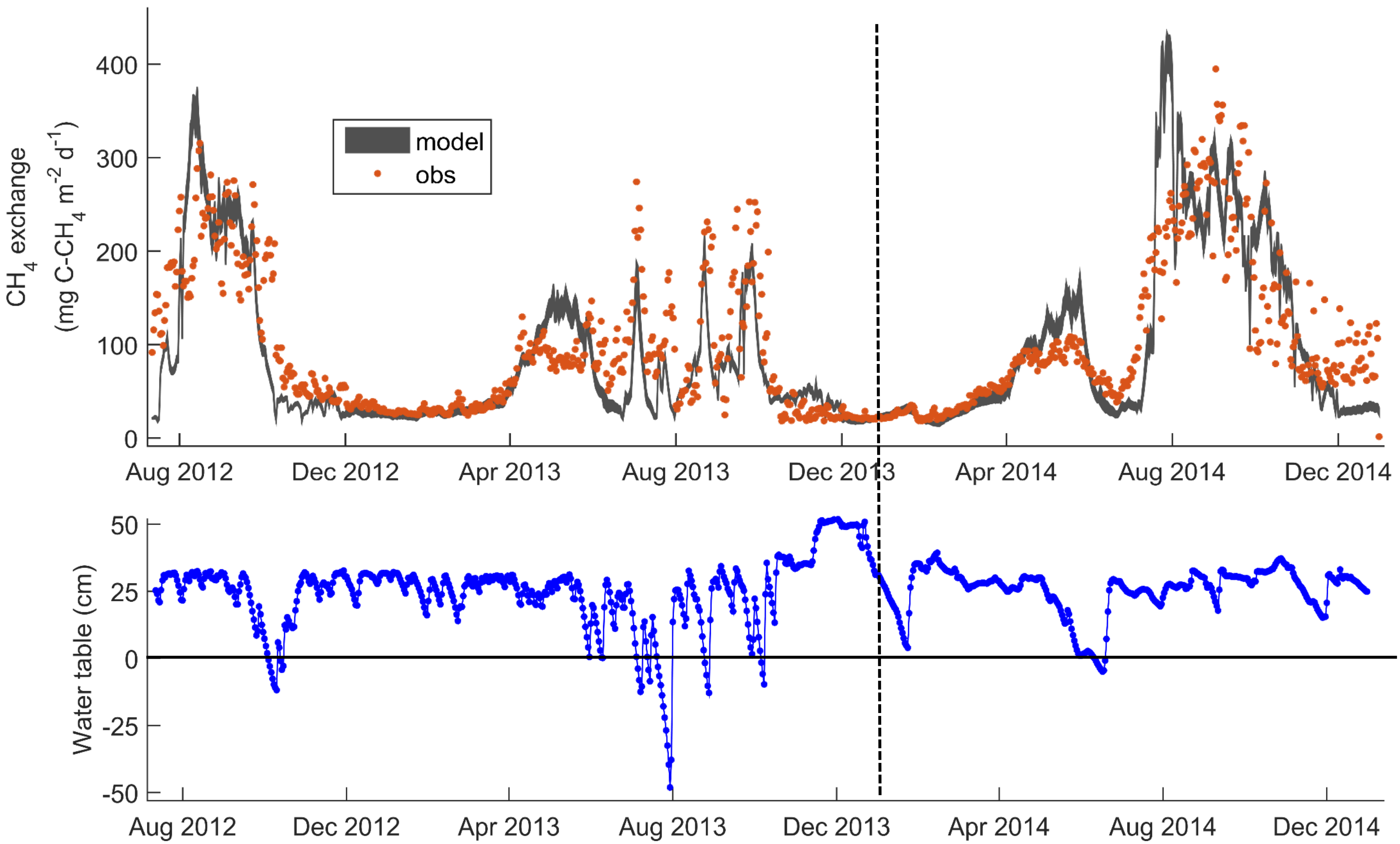
Oikawa et al. submitte



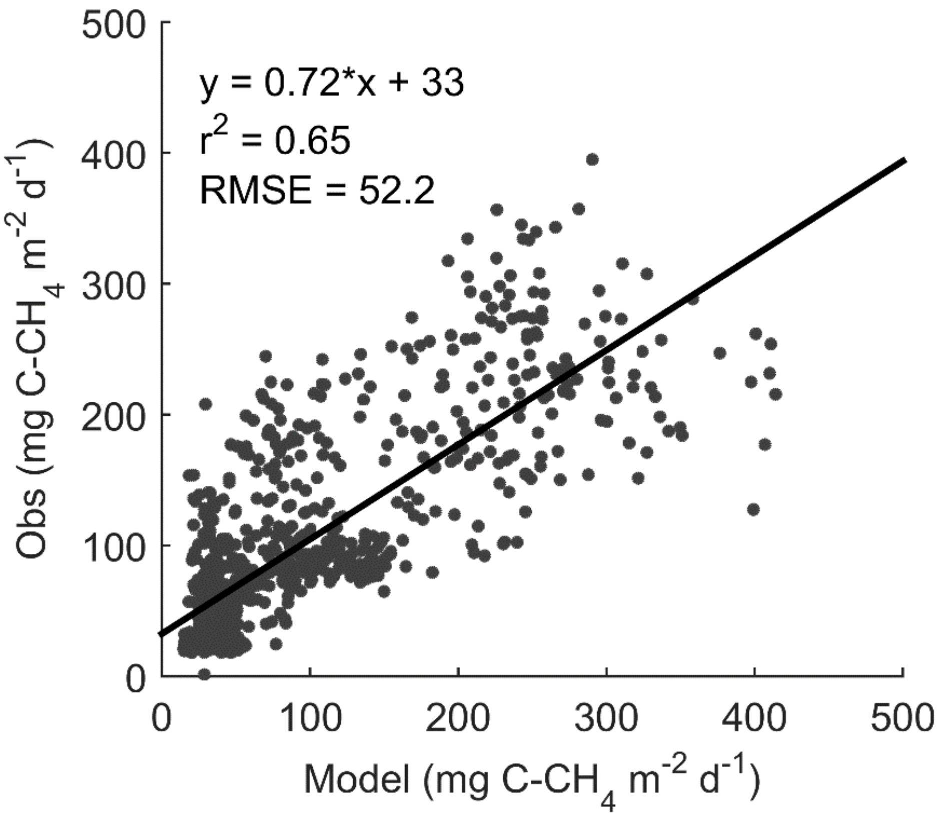


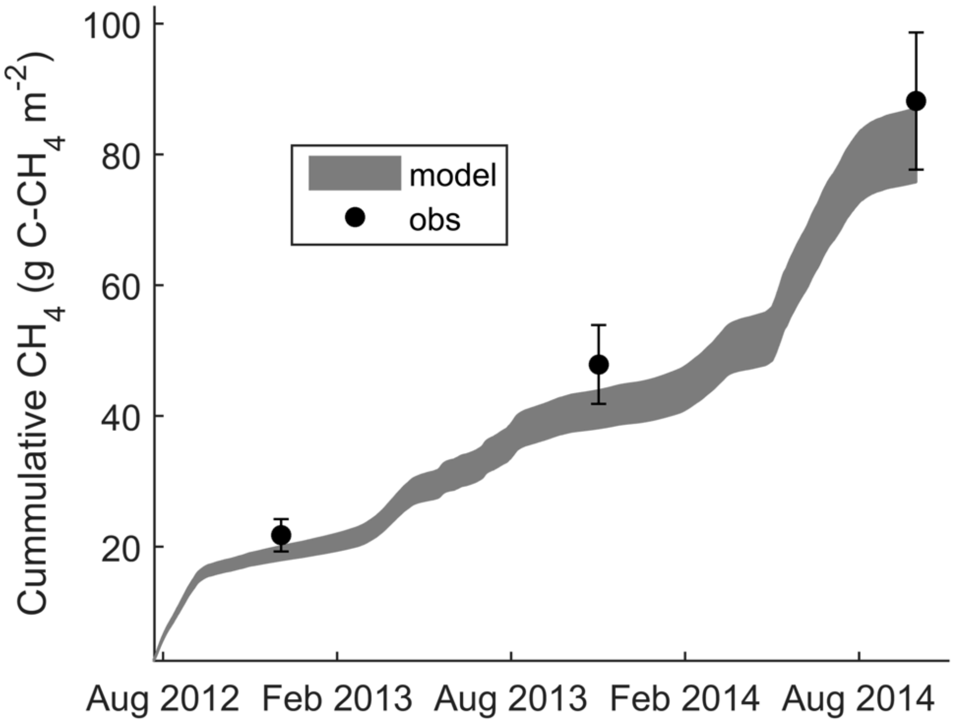
	Parameterization ($g\ CO_2\text{-}C\ m^{-2}$)	Validation ($g\ CO_2\text{-}C\ m^{-2}$)
Obs	- 931 ± 202	- 290 ± 134
Model	- 778 ± 152	- 329 ± 105

Oikawa et al. submitte



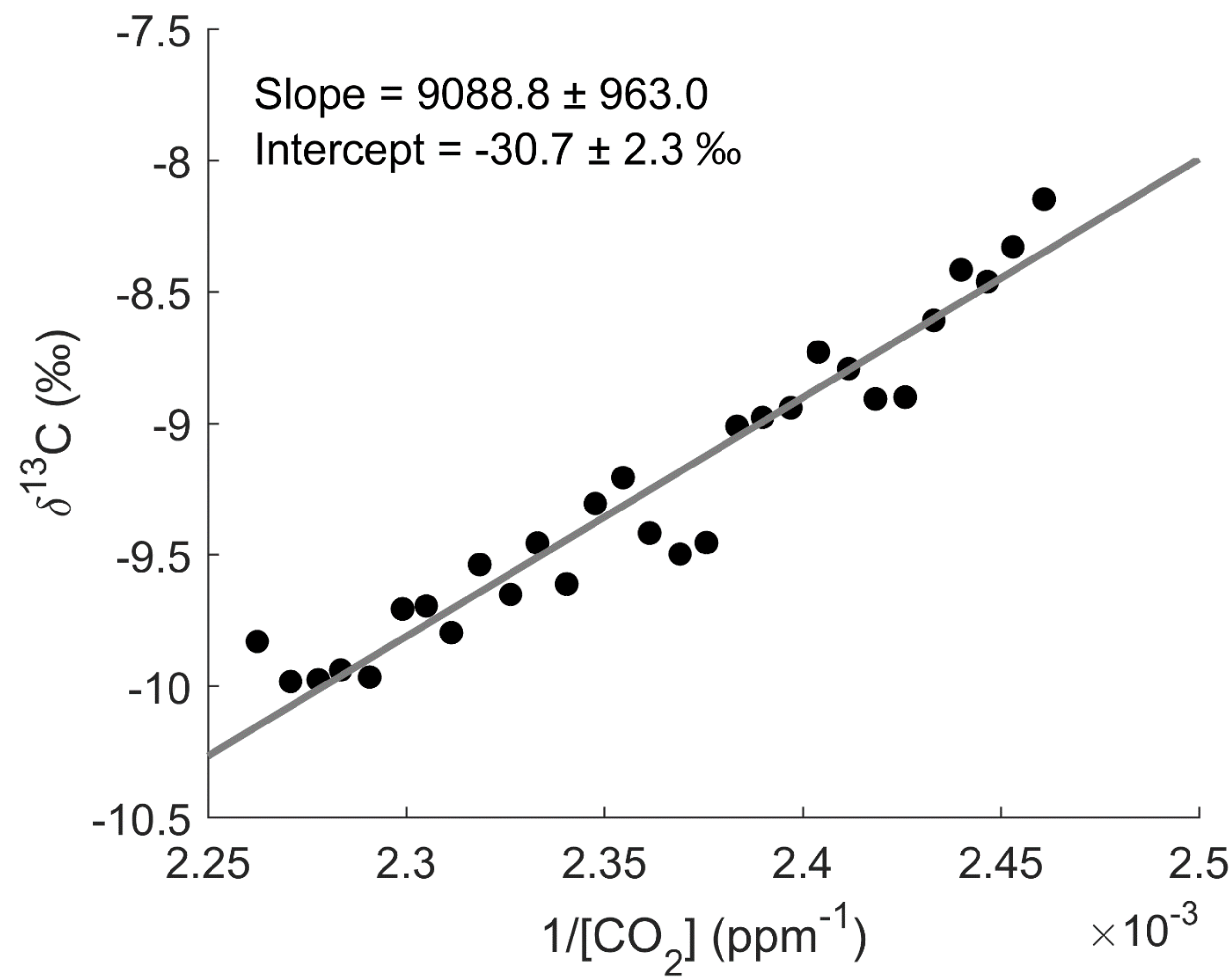
Oikawa et al. submitte





	Parameterization (g CH_4-C m^{-2})	Validation (g CH_4-C m^{-2})
Obs	48 ± 6	40 ± 4
Model	41 ± 3	40 ± 3

Oikawa et al. submitte


Slope = 9088.8 ± 963.0
Intercept = -30.7 ± 2.3 ‰
-7.5
-8
-8.5
-9
-9.5
-10
-10.5
δ13C (‰)
2.25
2.3
2.35
2.4
2.45
2.5
1/[CO2] (ppm-1)
×10-3

Venue: the Sacramento-San Joaquin River Delta

Can Be Expressed in Spectral Domain

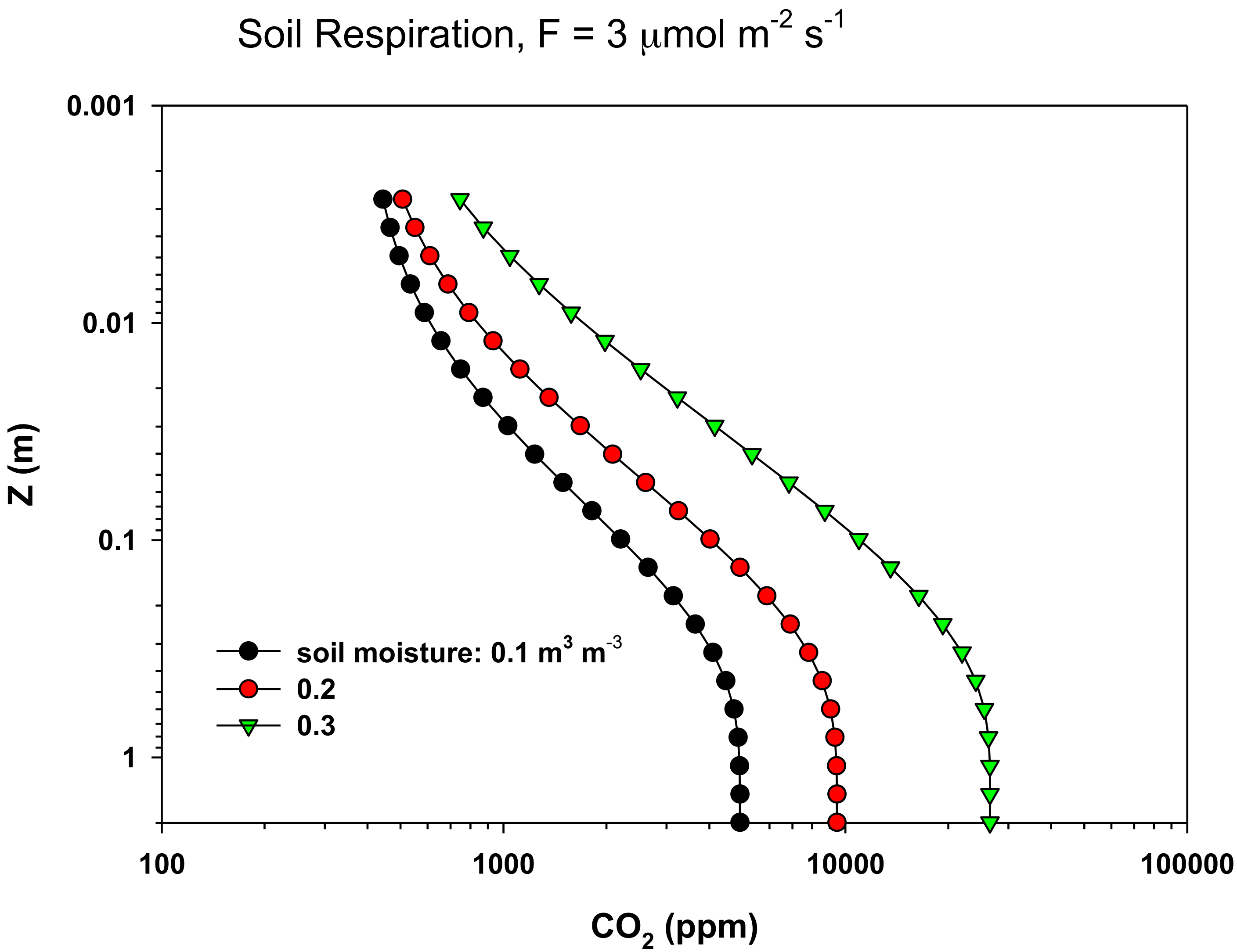
In frequency (f) domain:

$$I(f)_{y \to x} = \ln \left\{ \frac{S_{xx}(f)}{\mathrm{S}_{xx}(f) - [\boldsymbol{\Gamma}_{yy} - (\boldsymbol{\Gamma}_{xy}^2/\boldsymbol{\Gamma}_{xx})]|\mathbf{H}_{xy}(f)|^2} \right\}$$

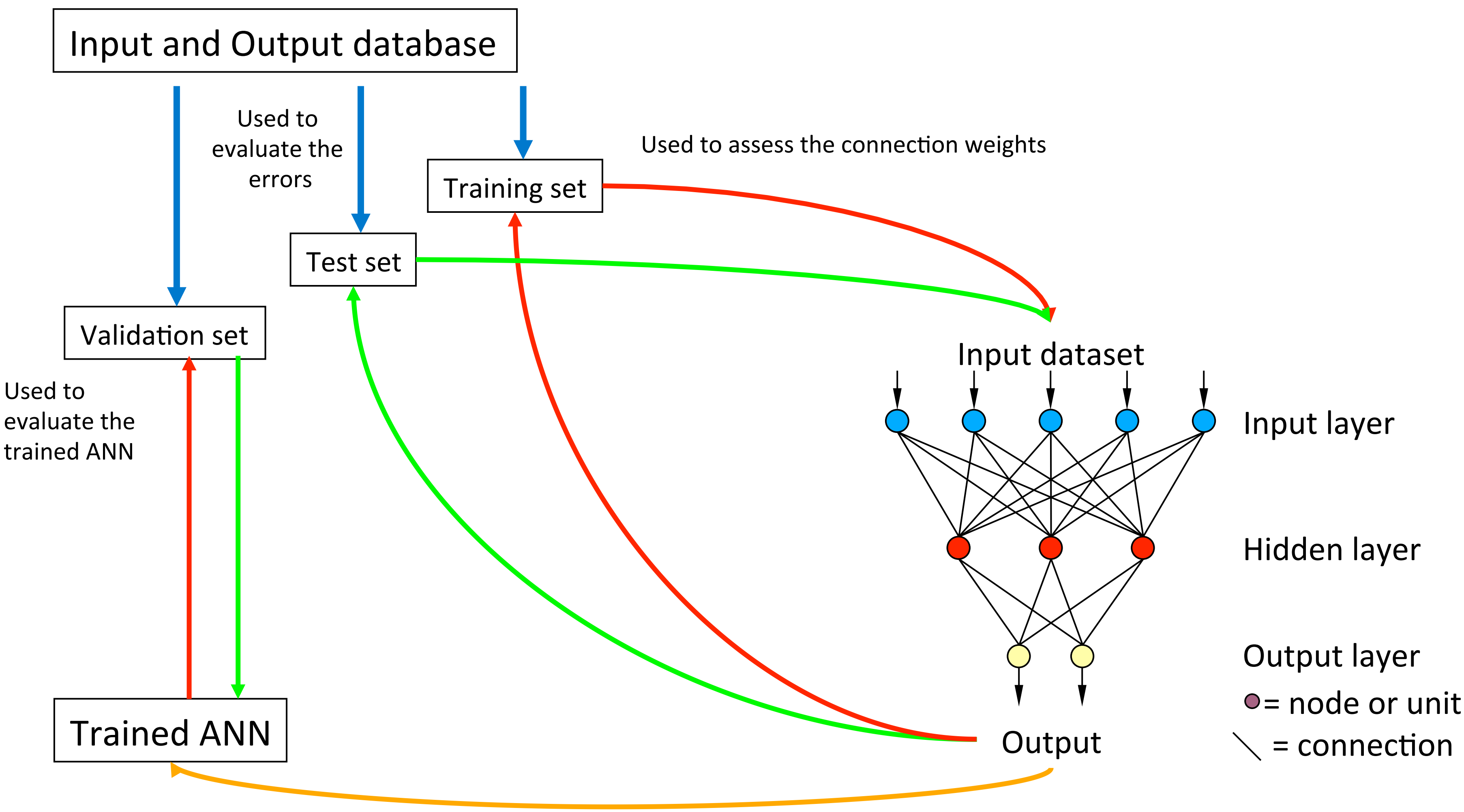
No interaction, $G \approx 0$
Interaction, $G > 0$

$S_{xx}(f)$ = power spectrum of x at frequency f
Γ = error covariance matrix of the bivariate model
H = transformation matrix from writing model in Fourier space

Using Models to Design Soil Respiration Studies



Artificial Neural Networks training



Slide courtesy of D Papale